DODECYLBENZENE HEALTH RISK ASSESSMENT ADDENDUM

DIAL CORPORATION MAIN FACILITY

SOUTH GATE, CALIFORNIA

Prepared for

Dial Corporation

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Prepared by

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Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
South Gate, California

The material and data in this report were prepared under the supervision and direction of the undersigned.

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1 INTRODUCTION

EMCON has completed this health risk assessment addendum for dodecylbenzene-impacted soil at the Dial Corporation (Dial) Main Facility, 9300 Rayo Avenue, South Gate, California (the Site). Dodecylbenzene-impacted soil was identified in the vicinity of the former Alkylate Unloading Area in the southwest corner of the Site.

To assess possible risk to groundwater and human exposure via inhalation and ingestion, a health risk assessment (HRA) was previously prepared and submitted by EMCON in January 1994 for dodecylbenzene-impacted soil at the Site (EMCON, 1994). Because toxicity and fate and transport values for DDB were not available, data from Monsanto for partially characterized mixtures of alkylbenzenes were used to supply the toxicological and transport parameters for assessing exposures and risks in the HRA. Results of the HRA indicated that levels of dodecylbenzene (DDB) detected in site soil did not pose an unacceptable health threat for potentially exposed receptors.

Comments on the HRA report were provided by the Regional Water Quality Control Board, Los Angeles Region (RWQCB), in a letter to EMCON dated February 13, 1996 (RWQCB 1996a). These comments included concerns about the toxicity values developed in the HRA for dodecylbenzene, and the fate and transport modeling assumptions used to evaluate the potential for dodecylbenzene to leach from soil to groundwater. In their comments, the RWQCB requested that a quantitative uncertainty analysis be performed on the reference dose and transport parameters used for DDB to assess the confidence in the conclusions reached in the HRA.

Because additional toxicological and fate and transport information on DDB or alkylate mixtures was not available, EMCON believed it advisable to explore other options for addressing RWQCB comments, including the need for a quantitative uncertainty analysis. A meeting was held on May 8, 1996, involving the RWQCB, Dial, and EMCON to discuss an alternative approach to addressing the RWQCB concerns. EMCON proposed an approach that involved implementation of a quantitative structure-activity relationship (QSAR) method using discrete chemicals (not mixtures) to develop a reference dose (RfD) and transport parameters for DDB. As proposed, published fate and transport and toxicity data for linear alkylbenzenes are extrapolated to provide input parameters for DDB modeling.

It was decided during the meeting that a workplan should be prepared to allow the RWQCB to fully review the approach prior to its implementation. A workplan outlining the approach was submitted to the RWQCB on June 5, 1996, and was accepted in principle by the RWQCB in their letter of August 16, 1996 (RWQCB 1996b). In this letter, the RWQCB requested that, in addition to the scope outlined in the workplan, that breakdown products of DDB be evaluated in the risk assessment. Theoretically, alkylbenzenes in the environment may break down to shorter alkylbenzenes or benzene. Benzene, toluene, and ethylbenzene were analyzed for in soil in the area where DDB was detected. Although the DDB was released to the environment over 10 years ago, these volatile degradation products have not been detected in soil samples collected from the area. This implies that degradation products which may be toxicologically important are not being produced at detectable levels, and no further evaluation of breakdown products is necessary.

Comment 4 from the RWQCB August 16, 1996 letter asked that we include the 95th cumulative percentile as a source concentration for dodecylbenzene in addition to using the 95 percent upper confidence limit of the mean (95UCL). Comparison of these values indicates that use of either value leads to the same conclusions in the risk assessment. Based on this information and because the 95UCL is recommended for use by Cal-EPA in risk assessments, the 95UCL was used in this addendum.

Comments 5 and 6 from the RWQCB August 16, 1996 letter asked that we include a range of input parameters into the SESOIL model rather than single values, and to conduct a sensitivity analysis of these ranges of values. These comments were based on the use of literature values in the original risk assessment. Since that time, additional site-specific data were compiled for use in the revised modeling task. Because inputs in the revised SESOIL modeling use actual site data, using a range of input values was no longer considered relevant. For the chemical parameters that did rely on literature information, the conservative ends of the ranges were used to maximize the possible movement of dodecylbenzene over time. Therefore, a sensitivity analysis (e.g., quantitative uncertainty analysis) was not conducted because the revised modeling was designed to maximize leaching.

In addition to these comments, an additional comment from the RWQCB February 13, 1996 letter not addressed in this Addendum relates to conducting an ecological risk assessment at the site. The site is in an industrial area adjacent to the Los Angeles river. No other habitats are located near the site due to the industrial development in the area. This river is a cement-lined, man-made water body that does not support aquatic habitat. Therefore, no ecological receptors are present near the site and no ecological risk assessment needs to be conducted.

This Addendum was conducted in accordance with the "Workplan for Risk Evaluation of Dodecylbenzene Using Quantitative Structure-Activity Relationships" (Workplan; EMCON, June 1996) and the "Proposal for Continuing Risk Assessment Services" submitted to Dial on August 22, 1996. Because this Addendum is intended to be an integral part of the HRA (EMCON, 1994), the reader is referred to the HRA for site and other information used to conduct the risk assessment. This Addendum provides the QSAR evaluation of fate and transport and toxicity values for dodecylbenzene, and using these data updates the SESOIL modeling and risk characterization results of the HRA report (EMCON, 1994).

A conceptual site model illustrating the transport potential of DDB at the site and possible exposure pathways for humans is provided as Figure 1-1. This figure is discussed in Section 2 below.

2 EXPOSURE ASSESSMENT

A QSAR approach was used to refine the modeling performed in the original HRA. The QSAR approach involves (1) the compilation of relevant chemical properties for the series of individual linear alkylbenzenes (i.e., toluene, ethylbenzene, propylbenzene, etc.), (2) examination of the variability of the properties with addition of -CH_2- (methylene) units to the alkyl chain, and (3) extrapolation of the structure-property relationship to DDB. The refined values of chemical properties for DDB obtained using this approach were used in SESOIL leaching and soil volatilization modeling.

Detected DDB levels were statistically evaluated in the vicinity of the former alkylate area to identify a concentration representing the 95 percent upper confidence limit (95UCL) on the arithmetic mean. This 95UCL was calculated to be 12,660 mg/kg using original site data. Based on the distribution of detected concentrations with soil depth, the upper ten feet of the soil column was represented for SESOIL modeling by a DDB concentration of 10,000 mg/kg, while the deeper ten feet (i.e., 10 to 20 feet bgs) was represented by 22,000 mg/kg. This is conservative for leachate modeling because a concentration greater than the 95UCL was placed deeper in the soil column. These concentrations were conservatively assumed to extend laterally over an area of 818 square feet (76 square meters).

SESOIL modeling had been performed before in the HRA using Monsanto data on Alkylate Mixture 215, and had supported the conclusion that DDB present in subsurface soils will not impact groundwater over a 25-year period. Alkylate 215 is a mixture of aromatic alkanes with alkyl chains ranging from 10 to 14 carbon atoms in length, one of which is DDB. Soil volatilization modeling had not been performed previously in the HRA and was conducted in this Addendum as requested by the RWQCB in February (1996a). This additional pathway is considered relevant to evaluate based on the conceptual site model (Figure 1-1).

2.1 Chemical Properties of DDB

A number of different sources of chemical properties for alkylbenzenes were consulted to compile the data used for the QSAR evaluation. Mackay's recent work (Mackay et al., 1992) provided the majority of the values; this source is up-to-date and contains multiple values for individual chemicals and parameters, and therefore provided a basis for evaluating the variability in the properties of linear alkylbenzenes.

Based on the input parameters needed to conduct SESOIL and soil volatilization modeling, values for four properties were compiled: water solubility, vapor pressure, Henry's Law constant, and organic soil-water partition coefficient (K_{oc}). Of these four properties, all but vapor pressure are used in SESOIL modeling to evaluate the downward leaching potential of DDB through vadose zone soils towards the water table; vapor pressure is a parameter used in soil volatilization modeling to evaluate the potential for DDB in the form of chemical vapors to diffuse upwards from the vadose zone and pose a potential inhalation hazard for the receptors evaluated in the risk assessment.

Although an effort was made to identify values for these parameters for as many alkylbenzenes as possible, the available data were scarce for alkylbenzenes with alkyl groups longer than four carbons (e.g., butylbenzene).

2.1.1 Properties of Alkylbenzenes

Tables 2-1 through 2-6 show the data compiled for toluene through hexylbenzene, as well as the sources of each value; no data were available for heptyl- or octylbenzene. For each parameter where at least four values were available, statistical tests were performed to characterize the datasets as either normally or lognormally distributed. The Shapiro-Wilk Test (W Test) was conducted for datasets containing between four values and 50 values. For datasets with more than 50 values, the D'Agostino's Test (D Test) was used. Both of these tests are described in Gilbert (1987).

The W Test computes a "W" statistic that, if the data are normally distributed, is larger than the lookup values found in Gilbert, 1987. The D Test computes a "Y" statistic that, if the dataset is normally distributed, is within the calculated range derived from information in Gilbert, 1987. If the datasets were not found to be normally distributed, the datasets were transformed logarithmically, then retested using the W or D Test as appropriate. A False positive rate of five percent was used for all tests in this evaluation.

In cases where the datasets could not be classified as either normally or lognormally distributed, the critical value closest to the lookup value (or Y range) was noted and the closer distribution was assumed. For example, for toluene solubility, the "D-Test range for Y" was closer to the "normal distribution" critical value, thus a normal distribution was assumed for this dataset. See Table 2-7 for dataset characterization test summary results.

Once datasets were characterized as "normal" or "lognormal" following this statistical procedure, arithmetic or geometric mean statistics were developed to identify the mean, the 95UCL, and the 5 percent lower confidence limit (5LCL). Of the 17 datasets tested, 10 could be characterized as normal and seven as lognormal (Table 2-7). Although the statistical tests performed for the partition coefficient dataset for toluene suggested that the dataset has more lognormal character than normal (Table 2-7), normal statistical results were used for the structure-property relationship, as the geometric mean for this dataset was calculated to be below the 5LCL (Table 2-1).

2.1.2 QSAR Analysis

Once the appropriate statistical values were obtained for each parameter dataset, the mean values were plotted against the number of methylene units in the alkylbenzene structure. For those chemical property datasets containing less than four data points, but more than one, values for the QSAR relationship evaluation were selected based on the following criteria:

- If a value was cited more than once by the sources consulted for the evaluation, that value was used (e.g., vapor pressure for pentylbenzene of .328 mmHg (Table 2-5).

- If no values were listed more than once, values were chosen to either maximize the impact of DDB on groundwater (i.e., parameters used for SESOIL modeling), or the impact on outdoor air (i.e., parameters used for soil volatilization modeling).

The results of the QSAR analysis for the linear alkylbenzenes are shown in Figures 2-1 through 2-4 for the mean values of the four properties. As Figures 2-1 and 2-2 show, water solubility and vapor pressure indicate strong inverse logarithmic relationships with length of the alkyl chain. A less clear relationship was observed for the partition coefficient (Figure 2-3), and no relationship was observed for the Henry's Law constant (Figure 2-4).

When the mean data points for each of the chemical property datasets were log transformed, very good straight-line behavior was observed for solubility and vapor pressure (Figures 2-5 and 2-6) when the log mean data points were plotted against alkyl chain length. A comparable Koc relationship was not clear from this data transform (Figure 2-7).

On the basis of these results, the water solubility and vapor pressure for DDB could be obtained from the existing data by standard regression fitting; values for the partition coefficient (K_{oc}) and the Henry's Law constant could be estimated based on the solubility and vapor pressure results for DDB rather than directly from the data provided in the tables. These methods and results are described in the following section.

Regression Analysis and Estimation of Properties for DDB. Table 2-8 presents the results of the simple linear regression analysis for water solubility and vapor pressure. As the results show, excellent regression fits are obtained for both parameters (r^2 of 0.976-0.997 for solubility and 0.999 for vapor pressure).

Table 2-9 shows the computations used to estimate values for the Henry's Law constant for DDB. The vapor pressure estimates for DDB (Table 2-8) were divided by the water solubilities at the three levels of statistical significance, which is a standard and well-accepted method for obtaining Henry's Law constant values (Lyman et al., 1990).

Table 2-10 shows the computations used to estimate values for the K_{oc}. The water solubility values estimated for DDB (Table 2-8) were used in a previously developed regression equation recommended by Cal-EPA in the Decision Tree manual (Cal-EPA, 1986), and also described by Lyman et al., 1990.

The chemical properties of DDB, as estimated according to the regression methods described in this section (Tables 2-8, 2-9, and 2-10), may be compared with values used in the original HRA based on the Monsanto data. For the water solubility, the values estimated in this Addendum are much lower than the value used in the previous HRA for SESOIL modeling input. The calculated values for the Henry's Law constant and the K_{oc} are much higher than what was used for modeling input in the previous HRA. These results mean that DDB should be less mobile with respect to leaching than what was previously modeled. SESOIL runs were performed using these estimated DDB properties along with site-specific, measured vadose zone properties, as requested by the RWQCB (1996a).

2.2 Revised Exposure Modeling

Estimated values for the four parameters described in the previous sections were used for groundwater impact and soil volatilization modeling. One additional parameter, the air diffusion coefficient, required for both types of modeling, was computed according to the molecular fragment method of Fuller, as described and recommended by USEPA (1988). Table 2-11 presents these calculations. The result of these calculations, 0.044 square centimeter per second (cm^2/sec), is very close to the value used in the previous HRA (0.045 cm^2/sec), suggesting that the same method was used by Monsanto in obtaining their value.

Groundwater impact (SESOIL) and soil volatilization modeling using these parameters are described in the following sections.

2.2.1 SESOIL Modeling

SESOIL modeling to evaluate the leaching potential of DDB was performed to address the comments of the RWQCB pertaining to the original risk assessment. In this additional evaluation of the leaching potential of DDB, the assumptions applied for SESOIL modeling in the original risk assessment were considered along with site-specific data on the soil characteristics in the area of concern (Appendix A). These site-specific parameters were combined with the chemical-specific parameters discussed in the previous sections to refine the SESOIL modeling.

SESOIL is a sophisticated, computerized model developed for USEPA in 1987 (GSC, 1987). SESOIL conserves chemical mass and considers both the upward loss of soil chemicals due to volatilization, and the downward transport in the condensed and aqueous phases. SESOIL is a seasonal soil compartment model that estimates the rate of vertical chemical transport and transformation in the soil column in terms of mass and concentration distributions among the soil, water, and air phases in the unsaturated soil zone, as well as estimating the mass of chemical flow into groundwater. The SESOIL program used in the current evaluation is RISKPRO's SESOIL for Windows Version 2.5, which uses a convenient Windows-based interface for entering all SESOIL inputs and selecting an appropriate meteorological dataset from the program's climate database.

The latitude and longitude of the Los Angeles Airport (lat: 33-56-33.130N, long: 118-24-29.068W) was used to select an appropriate meteorological station database from the SESOIL program, since the site is in the general vicinity of the airport. The "Los Angeles WSO AP", the closest station to LAX (1.3 kilometers), was used in the current evaluation. Rainfall events at the site were not adjusted for the presence of asphalt because this has recently been removed from the site.

An evaluation of the two boring logs for locations EB-2 and EB-3 showed two differences between the soil column configuration used in the original SESOIL model and the current evaluation:

- There is a relatively impermeable soil layer with a high clay content occurring at about 21 to 31 feet bgs; the original evaluation conservatively assumed a clay content of zero percent

- The depth to groundwater has been as shallow as 37 feet bgs; the original evaluation assumed a depth of 57 feet bgs

In addition to these differences, the properties for DDB used in the model were different than those used originally, as requested in RWQCB comments. The properties developed for DDB in the previous section indicate that DDB is substantially less mobile than assumed in the original assessment, even using 95UCL properties developed in this evaluation rather than mean values. Because 95UCL values were used for chemical-specific properties, a sensitivity analysis on these parameters was not considered appropriate. However, comparison of mean and 95UCL values and SESOIL outputs using both sets of values indicates that the impact of these parameters on the modeling results are negligible.

The soil boring logs shown in Appendix A suggest that three soil layers may be identified for the subsurface lithology of the vadose zone:

- a silty sand layer extending from the surface down to about 21 feet bgs
- a sandy clay layer occurring from about 21 to 31 feet bgs
- a silty sand layer from about 31 feet bgs to the top of the water table at about 37 feet bgs.

Because the incorporation of DDB in the model previously assumed in the original evaluation divided the top 20 feet of the soil column into two layers, the 21-foot shallow layer described above was divided into two layers, each with the same soil properties but containing different DDB concentrations, as previously discussed. Therefore, a total of four layers was used for DDB leachate modeling, the same number of layers used in the previous HRA, as summarized below:

- 0 to 10 feet bgs, silty sand, 10,000 mg/kg DDB
- 10 to 21 feet bgs, silty sand, 22,000 mg/kg DDB
- 21 to 31 feet bgs, sandy clays, no DDB
- 31 to 37 feet bgs, silty sands, no DDB

As required by the model, sublayers were identified for each of the four major layers as follows:

- Layer 1, 0 to 10 feet bgs, 10 sublayers
- Layer 2, 10 to 21 feet bgs, 10 sublayers
- Layer 3, 21 to 31 feet bgs, 10 sublayers
- Layer 4, 31 to 37 feet bgs, 1 sublayer

The use of sublayers is intended improve the resolution of the model. Once the configuration of the model was established, vadose zone properties were selected based on the soil lithologies described above. Based on the model requirements, two main types of soil properties were identified:

- Layer-specific properties
- Vadose-zone properties (one value for the entire soil column)

In the latter case, weighted average inputs across depths were used. The selection of these soil property values is described in the following sections.

Vadose Zone Properties. Although physical analysis of soil samples taken from borings EB-2 and EB-3 provided values for several critical soil properties, special input requirements of the SESOIL model precluded direct use of two of these soil properties: permeability and porosity. For instance, although true soil permeabilities were obtained for the site, SESOIL requires the use of "intrinsic" permeabilities. The conversion of a site-specific true permeability to an intrinsic permeability entails considerable uncertainty. Therefore, another "site-specific" approach was taken to obtain usable input values for SESOIL for these two parameters. Recommended values for these soil properties contained in the SESOIL program software were matched against the known soil types obtained from the boring logs for the various model depth layers. This method is described in more detail below.

Intrinsic permeability

Unlike most other soil parameters, intrinsic permeabilities may be entered into SESOIL as layer-specific values. The SESOIL recommended values for loamy sands and sandy clays are 5×10^{-8} and 1.5×10^{-9} square centimeters (cm^2), respectively. These values were used as inputs for Layers 1,2, and 4 and Layer 3, respectively, based on the boring logs from the site.

Effective porosity

Values for effective porosities for loamy sands (0.28) and sandy clays (0.24) provided in the SESOIL software were used to compute a weighted average value of 0.27, which was used in the current evaluation for the entire vadose zone. SESOIL uses one value to represent the entire soil column.

Soil density

The soil boring log for EB-2 shows a density of 90 pounds per cubic foot (lbs/ft^3) for the silty sands in the lowest layer. Assuming this value also represents the top two silty sand layers results in a total of 27 of the 37 foot vadose zone having a density of 90 lbs/ft^3. For layer 3, the sandy clay layer, boring logs for EB-2 and EB-3 indicate a range of 86 to 93 lbs/ft^3. An average of 89 lbs/ft^3 was used to represent the density for this 10-foot layer. SESOIL uses one value to represent the entire soil column for this parameter. Calculating a weighted average soil density from these data results in a value of 90 lbs/ft^3 for the entire vadose zone. Converting units gives 1.43 grams per cubic centimeter (g/cm^3). This value may be directly compared with the value of 1.35 g/cm^3 used in the previous HRA.

Disconnectedness index

A value for this parameter could not be identified from the soil boring log data presented in Appendix A. The SESOIL software provides a recommended range of 3.7 to 12 for this parameter for sands to fine clays. A value of 3.9 is listed for loamy sands and 6 for sandy clays. No value is provided for silty sands. A weighted average value of 4.5 was computed and used in the current evaluation for the entire vadose zone using the same approach taken for the soil density parameter.

Percent organic carbon

Although total organic carbon (TOC) was measured for both boring locations EB-2 and EB-3, SESOIL requires a percent organic carbon. A value of 0.1 percent organic carbon was used in the current evaluation. Cal-EPA has recommended a conservative default value of 2 percent organic carbon (California, 1994), which is 20 times higher than the value used in the current evaluation. Since a lower organic carbon content will overestimate the impact to groundwater, the use of the 0.1 percent value should be considered conservative.

Cation exchange capacity

A value of zero was input, as DDB is an uncharged organic compound.

Freundlich Equation exponent

A default value of 1 was used, as recommended by the SESOIL program, in the absence of site-specific information for this parameter.

Other Input Parameters. To address comments from the RWQCB, the extreme confidence limits of the chemical-specific parameters developed in the previous section were used to re-evaluate the leaching potential of DDB. That is, the high end of the water solubility (0.0012 mg/L), the low end of the Henry's Law constant (0.05 atm-m^3/mol), and the low end of the Koc range (7.3 x 10^5 L/kg) were used. Using these extreme values for all three of these chemical-specific inputs represents a considerable degree of conservatism in the overall modeling approach. Additionally, SESOIL simulation was extended out to 99 years from the 25 year-period used in the original assessment.

Results of SESOIL modeling. The complete results of SESOIL modeling are included in a diskette attached to this report (Appendix B). The original file has been compressed using the "pkzip" utility. The original file may be recovered by using the "pkunzip" utility, also included on the diskette.

Figure 2-8 graphically shows the results of revised SESOIL modeling. As the figure shows, the downward movement of DDB is barely discernible over the 99-year simulation period, whereas the original evaluation predicted a downward movement for DDB of six feet towards the water table. This is particularly significant in light of the degree of conservatism associated with the chemical parameters used in concert with the site-specific data for some soil-based parameters. Some of the main conservative assumptions used in the model include:

- Use of extreme confidence limit values for the chemical-specific parameters
- Assumption of no chemical degradation over the 99-year period
- Assumption that all site soils are exposed to rainfall without attenuation from structures, vegetation, or pavement over a 99-year period

Considering the results of revised SESOIL modeling along with these conservative assumptions, it is concluded that the DDB still present in site soil should have no impact on groundwater beneath the site.

2.2.2 Volatilization Modeling

Because of the high soil DDB concentration assumed for the site (greater than 12,000 mg/kg), it was necessary to use a Raoult's Law-based volatilization model (for saturation concentrations). Although SESOIL contains a volatilization component, which it runs to conserve mass in estimating downward migration, this component is more appropriate for soils that contain lower concentrations of COPCs, and likely underestimates the vapor emission potential of a chemical. Therefore, a simple calculation based on Shen's model (Shen, 1981; as recommended by USEPA, 1988) was conducted and is shown in Table 2-12. Shen's model is generally regarded as providing relatively conservative estimates of the vapor emissions of chemically-impacted soils. It was assumed that a clean layer of soil 2 ½ feet thick overlies the deeper DDB contamination, and provides some retardation of upward vapor migration. This is a reasonable assumption, since available site data (EMCON, 1992, 1993a,b) show that detectable levels of DDB are deeper than 5 feet bgs.

The output from Shen's model, a chemical vapor flux at the soil surface, was then input into a simple and conservative box model to estimate an air concentration above the contaminated soil (Cal-EPA, 1994; USEPA, 1991, 1996a). Table 2-13 shows the computation used to estimate an outdoor air concentration of DDB from soil emissions. The input parameters for the box model are the same as those used to estimate an outdoor chemical dust concentration in the HRA. An outdoor vapor concentration of 1.5×10^{-7} milligrams per cubic meter (mg/m^3) DDB was obtained. This concentration was used in Section 4, along with the result of the toxicological evaluation (Section 3), to estimate a noncarcinogenic hazard quotient for the vapor inhalation pathway.

3 TOXICITY ASSESSMENT

In this section, a quantitative structure-activity relationship (QSAR) approach is conducted to develop an RfD for DDB. This RfD will be compared with estimated exposures to evaluate the possible hazards to human receptors from exposure to DDB.

The concept behind the QSAR approach is that structurally similar compounds have similar mechanisms of action. Toxicological information available on some compounds in a group can be extrapolated to other chemicals in the group. A chemical's structure, solubility, stability, pH sensitivity, electrophilicity, and chemical reactivity can provide important information for use in hazard identification and risk assessment. This approach has been used by the U. S. Environmental Protection Agency (USEPA) and the State of California to develop toxicity equivalence factors (TEFs) for dioxins (USEPA, 1994) and polycyclic aromatic hydrocarbons (PAHs) (USEPA, 1993). The approach is also used for meeting deadlines responding to premanufacturing notices for new chemical manufacture under the Toxic Substances Control Act (TSCA; Faustman and Omenn, 1996). As stated in the USEPA's revised proposed guidelines for carcinogen risk assessment (USEPA, 1996b), the predictive capability of QSAR has been documented. To support this claim, the USEPA recently used the QSAR approach to develop comparative slope factors for coplanar polychlorinated biphenyls (PCBs) (USEPA, 1996c). As discussed by the USEPA (1996b), the following information is useful for conducting a QSAR:

- Nature and reactivity of physiologically active portion of a chemical
- Mechanism of toxic action
- Physicochemical properties
- Structural and substructural features (e.g., stearic hindrance)
- Metabolic pathway (e.g., activation:detoxification ratio)
- Exposure route

The major shortcoming of the QSAR approach is in predicting activity (e.g., toxicity) across classes of chemicals and across multiple toxic endpoints using a single biological response. Because DDB is in the same chemical class as benzene, toluene, ethylbenzene, and other chemicals that have similar mechanisms of action for noncancer effects, the effects of this shortcoming on the present study should be minor, as further discussed below.

3.1 General Approach

Due to the lack of available toxicity data for DDB (EMCON, June 1996), a QSAR approach based on data for various alkylbenzenes was used to estimate an oral RfD for DDB. Data for different chemicals on the same exposure route and test species are needed to conduct a QSAR evaluation. Currently, the most relevant route of exposure to DDB at the site is via inhalation, although direct contact may be possible if invasive activities occur at the site. Data on both inhalation and oral exposure routes were evaluated in the literature, but only sufficient oral toxicity studies were identified in the literature that met the above criteria. Therefore, the RfD developed using this approach will be most relevant for oral exposure. In the absence of sufficient information on the inhalation route, this oral RfD will also be used to approximate an inhalation RfD, consistent with California Environmental Protection Agency (Cal-EPA) guidance (i.e., route-to-route extrapolation). The same values were used for both oral and inhalation RfDs for DDB provided previously (EMCON, 1994), so the assumption of equivalent toxicity via both routes is valid for this QSAR analysis. Information previously compiled and presented regarding the likely carcinogenic potential of DDB indicates that it does not act as a possible or probable human carcinogen (EMCON, 1994). Therefore, this analysis is restricted to evaluation of noncancer effects of DDB.

The first step in the QSAR evaluation is to compile oral LD_{50} data for various alkylbenzenes in the same species. A "best fit" equation is then developed for the relationship between structure (i.e., the effect of adding additional CH_2 units on the aromatic ring) and LD_{50} toxicity. This relationship is used to estimate an LD_{50} value for DDB. One oral rat study on DDB is available in the literature (Clayton and Clayton, 1982, as cited in the hazardous substances data bank, HSDB 1996) and will be used to compare with the value estimated using the QSAR approach.

The estimated LD_{50} for DDB is then converted to a no-observed adverse effect level (NOAEL) using information relating LD_{50} values and NOAELs from Layton et al. (1987) and Lewis et al. (1990). Once a NOAEL has been fully developed for DDB, USEPA uncertainty factors and metabolic scaling factors (USEPA, 1996b) may be applied, if necessary, to convert this rat-based NOAEL to a human-equivalent RfD.

A literature search was conducted to locate the relevant LD_{50} toxicity studies, which were used as the basis for a RfD for DDB. The following sources were consulted:

- Sax's Dangerous Properties of Industrial Materials (Lewis, 1992)
- Handbook of Environmental Data on Organic Chemicals (Verschueren, 1983)

- The Merck Index (Merck, 1989)
- Integrated Risk Information Service (IRIS; USEPA, 1996d)
- Registry of Toxic Environmental Chemical Substances (RTECS, 1996)
- Hazardous Substances Databank (HSDB, 1996)
- USEPA Health Advisories (chemical-specific)
- Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles (chemical-specific)

The open literature was also consulted, including a query on the internet (October 21, 1996), to identify additional information and data relevant to this work.

3.2 Lethal Toxicity Data for Alkylbenzenes

Information on oral rat LD_{50} values was available for alkylbenzenes ranging from one to four methylene ($-CH_2-$) groups in length (DDB contains a 12-carbon alkyl chain). This information is summarized on Table 3-1. A range of LD_{50} values was reported for benzene (930 to 3,400 mg/kg), toluene (2,600 to 7,300 mg/kg), and ethylbenzene (3,500 to 5,460 mg/kg). A single value was available for propylbenzene (6,040 mg/kg). No LD_{50} values were available for butylbenzene, but an LDLo of 5,000 mg/kg was reported (Table 3-1). The LDLo represents the lowest concentration at which any deaths to dosed animals occurs. The concentration at which 50 percent of the animals would die (i.e., LD_{50}) is higher than this value, but was not reported in the study (RTECS, 1996). Observing a range of LD_{50} values for a given chemical is typical when studies are conducted by different laboratories. Rather than take an average of the LD_{50} values for a given chemical, the lowest LD_{50} value was conservatively selected to represent the lethality of each alkylbenzene. These lowest LD_{50} values are shown below and on Table 3-1:

- Benzene 930 mg/kg
- Toluene 2,600 mg/kg
- Ethylbenzene 3,500 mg/kg
- Propylbenzene 6,040 mg/kg

As is evident from these values, the LD_{50} appears to increase as the length of the alkyl chain attached to benzene increases. These values appear consistent with respect to the LD_{Lo} of 5,000 mg/kg reported for butylbenzene. In addition, an LD_{50} value is available from Monsanto (1993) for the Alkylate 215 mixture. The Alkylate 215 mixture is reported to be comprised of the following (Robinson and Schroeder, 1992):

- 21.43 percent C10 alkylbenzenes (i.e., alkylbenzenes with 10-carbon alkyl chains)
- 42.6 percent C11 alkylbenzenes
- 35 percent C12 alkylbenzenes
- 0.74 percent C13 alkylbenzenes

DDB represents one of the C12 alkylbenzenes contained in Alkylate 215. Both straight-chain and branched alkanes are likely present in the mixture. Branched chain alkanes tend to be more toxic than straight-chained alkanes, so the toxicity of the mixture is likely to be greater than the toxicity of the linear alkylbenzenes for these carbon lengths. The LD_{50} value reported by Monsanto (1993) for Alkylate 215 is 17,000 mg/kg. More than half of the total mixture is comprised of C11 or smaller alkylbenzenes. This LD_{50} value was assumed to be reflective of a C11 straight-chain alkylbenzene. This is a conservative assumption for the following reasons:

- Alkylate 215 is a mixture including branched alkylbenzenes, which are generally more toxic than straight-chained alkylbenzenes.
- The average carbon length in Alkylate 215 is greater than 11.0, so the toxicity represents a mix of alkylbenzenes longer than C11.

A regression analysis using the lowest LD_{50} values presented above for benzene, toluene (one CH_2 group), ethylbenzene (2 CH_2 groups), propylbenzene (3 CH_2 groups), and Alkylate 215 (11 CH_2 groups) is provided on Figure 3-1. The R^2 value for this analysis is 0.996, indicating a good straight-line fit of the values. This indicates that addition of CH_2 groups to the benzene molecule lowers the acute toxicity of the alkylbenzenes by a predictable amount across the range of alkyl groups evaluated. Extrapolation of the line generated by the regression analysis to a C12 alkyl length results in an estimated LD_{50} value of 18,500 mg/kg for DDB.

To provide perspective on this estimated DDB LD_{50} value, the oral lethality study of DDB in rats conducted by Clayton and Clayton (1982) stated that " . . . 5 g/kg [5,000 mg/kg] caused no deaths . . . ." The LD_{Lo} would therefore be greater than 5,000 mg/kg, and the LD_{50} greater still. In addition, the estimated LD_{50} value for butylbenzene extrapolated from the regression line is approximately 7,500 mg/kg. Considering the LD_{Lo} reported for butylbenzene is 5,000 mg/kg, the extrapolated LD_{50} value is a plausible estimate of the LD_{50} value for butylbenzene.

This LD_{50} value for DDB of 17,500 mg/kg is converted to a chronic NOAEL for use in developing an oral RfD as discussed below.

3.3 Conversion of Lethal Value to NOAEL

Several approaches have been recommended to extrapolate LD_{50} values to NOAELs. Approaches vary in their degree of conservativeness. Three of these approaches are briefly discussed below, in increasing levels of conservativeness.

3.3.1 Lewis et al. (1990) Studies

Lewis et al. (1990) evaluated chemical-specific ratios between LD_{50} values and no-observed effects levels (NOELs) for the same species in a total of 490 studies. A NOEL is different from an NOAEL in that the former identifies any change in the animal, not just those considered "adverse". This comparison provides an evaluation of the relationship between a NOEL and an LD_{50} for use in developing an appropriate uncertainty factor to extrapolate from an LD_{50} to a NOEL. On the basis of the results obtained by Lewis et al. (1990), lowering the LD_{50} by a factor of 6 appears to be sufficiently protective for individuals within the population, including sensitive individuals. Because LD_{50} data are based on acute studies, the NOEL extrapolated from such data should be considered to be a short-term (e.g., acute) NOEL. The acute NOEL must then be adjusted to an equivalent chronic daily NOEL using an appropriate uncertainty factor. Although USEPA uses a value of 10 for this adjustment (i.e., acute to chronic), information provided in Lewis et al. (1990) indicates a value of 5 is sufficient. Therefore, a range of uncertainty factors between 30 (5 x 6) and 60 (10 x 6) can be used to adjust an LD_{50} value to an equivalent chronic NOEL using the approach of Lewis et al. (1990). This results in a range of chronic NOAEL values for DDB of 308 to 615 mg/kg/day. This is consistent with the data provided by Layton et al. (1987), who calculated a geometric ratio between chronic rat NOELs and LD_{50} values of 66.

3.3.2 Edmisten Watkin and Stelljes (1993) Study

A similar approach developed from the Lewis et al. data along with data compiled by McNamara (1979) was presented by Edmisten Watkin and Stelljes (1993) specifically for use in extrapolating toxicity values across mammalian species. This approach uses the same factor of 6 to extrapolate from an LD_{50} value to an acute NOEL, but incorporates an additional safety factor in recognition of the possibility that the target species (in this case humans) may be more sensitive to the toxicity of a chemical than the test species (rats in this case). Using this approach, the following extrapolation factors are recommended in addition to the factor of 6:

- A factor of 5 to extrapolate from short-term to a chronic basis
- A factor of 20 to extrapolate from a test species in a different family than the target species
- A modifying factor of 10 to account for the lack of sublethal data on the alkylbenzenes

Therefore, using this approach, a total extrapolation factor of 6,000 (6 x 5 x 20 x 10) is suggested to convert the estimated DDB LD50 value to a chronic NOAEL. This results in an oral chronic NOAEL of 3.1 mg/kg/day for DDB.

3.3.3 Layton et al. (1987)

A third approach was recommended by Layton et al. (1987), who developed the approach specifically to provide provisional, conservative chronic acceptable daily intakes (now known as reference doses) for humans in the absence of nonlethal data. They conducted statistical analysis to develop ratios of chronic NOELs and LD_{50} values for many chemicals in rats, and further evaluated impacts of interspecies variability on these ratios. In addition, they compared ratios of acceptable daily intakes and LD_{50} values for 96 pesticides derived by the World Health Organization (WHO) and Food and Agricultural Organization (FAO) of the United Nations. The results of their analyses indicated the following:

- Lower-bound estimates of a chronic NOEL can be made by multiplying an oral LD_{50} for small mammals by a factor ranging from 5×10^{-4} to 1×10^{-3}. This is equivalent to dividing the LD_{50} value by a factor ranging from 1,000 to 2,000.
- To estimate a conservative, interim RfD, the oral LD_{50} values can be multiplied by conversion factors ranging from 5×10^{-6} to 1×10^{-5}. This incorporates an additional safety factor of 100, resulting in a range of extrapolation factors from 100,000 to 200,000.

Using this approach and including the additional safety factor of 100, a total extrapolation factor of 100,000 to 200,000 could be used, resulting in a range of RfDs from 0.09 to 0.018 mg/kg/day. These RfDs should provide extremely conservative estimates of a chronic NOAEL for DDB, as intended by the authors.

3.3.4 Summary

These approaches all utilize the uncertainty factor or safety factor method for developing RfDs, which was formally developed by Dourson and Stara (1983). In this original approach to safety factors, values of 10 were arbitrarily used to adjust toxicity values downward to be protective of humans. The reason for this approach is that, when these factors were first suggested in 1954, information on comparative toxicity was scarce (Lehman and Fitzhugh, 1954). Therefore, factors of 10 were used to incorporate margins of safety for different extrapolations rather than be reflective of the actual differences in toxicity using toxicity tests. More recently (Dourson et al. 1996), it has been suggested that these order-of-magnitude factors should be regarded as upper-bounds on these extrapolations and that the combination of 10-fold uncertainty factors greatly overestimates the actual toxicity of many chemicals. As stated by Dourson et al., (1996), ". . . ultimately the goal of risk assessment is . . . to be able to describe the risk, or lack of risk, posed by various exposures with as little uncertainty as possible." The authors conclude by recommending that the default should be to embrace the use of data-derived uncertainty factors, and 10-fold factors should only be used in a situation where " . . . there is truly inadequate data . . . ." The USEPA has begun using less than 10-fold factors for extrapolations within a species, across species, from less-than-chronic to chronic exposures, from low-effect levels (LOELs) to NOELs (Dourson et al., 1996).

Based on this discussion, values ranging from 30 to 200,000 can be used to convert the acute LD_{50} value of DDB to a chronic human-based RfD. The most conservative RfD resulting from these approaches is 0.09 mg/kg/day and the least conservative RfD is 615 mg/kg/day. Data available on alkylbenzenes for sublethal endpoints are presented in the following section to identify, using actual data, an appropriate uncertainty factor to derive an oral RfD for DDB.

3.4 Development of Oral RfD

Table 3-1 summarizes toxicity on nonlethal endpoints for alkylbenzenes in rats and mice. Although oral subchronic and chronic data were scarce, subchronic oral toxicity studies were available for benzene, toluene, ethylbenzene, and Alkylate 215 mixture. A comparison of the LD_{50} values with NOAELs for the same species and chemical can be useful in determining an appropriate uncertainty factor with which to derive an RfD. Using the lowest LD_{50} values reported in the table, the ratio of LD_{50} values to NOAELs can be summarized as follows:

Chemical	Ratio
Benzene	930
Toluene	4.4
Ethylbenzene	12
Alkylate 215	3,400

Although this is a wide range of ratios, the highest ratio of 3,400 is much less than the highest uncertainty factor of 200,000 identified in the previous section. One reason for the wide range of ratios is that different sublethal endpoints were evaluated. For example, the endpoint evaluated for Alkylate 215, which had the highest ratio, was reproductive effects, which typically are more sensitive endpoints than non-reproductive endpoints. At the other end of the spectrum, the endpoint evaluated for toluene represented toxicity in three different organ systems (liver, kidney, and blood). To be adequately conservative, therefore, an extrapolation factor no less than 3,400 should be used to convert the LD_{50} to a human RfD.

Use of an extrapolation factor of 3,400 results in an oral RfD of 5.4 mg/kg/day. Use of the maximum extrapolation factor of 200,000 identified in the previous section results in an oral RfD of 0.09 mg/kg/day. The RfD used previously for dodecylbenzene was 0.05 mg/kg/day (EMCON, 1994), which adopted the 100-fold margin of safety to the subchronic NOAEL of 5 mg/kg/day reported for reproductive effects of Alkylate 215 (Table 3-1). Based on this analysis, the previously developed value of 0.05 mg/kg/day should be considered an upper-bound on the potential chronic, sublethal toxicity of DDB. The most conservative value derived through use of the QSAR methodology and data-derived extrapolation factors of 0.09 mg/kg/day should therefore be adequately protective, and perhaps overly protective, of human health and is adopted for use in this Addendum. To provide additional comparison, the oral RfDs for toluene and ethylbenzene are 0.2 and 0.1 mg/kg/day, respectively (USEPA, 1996d). The proposed conservative RfD for DDB is less than these values even though the data indicate that toxicity of linear alkylbenzenes declines with increasing length of the alkyl chain.

The calculations and resulting oral RfD for DDB are presented on Table 3-2.

4 RISK CHARACTERIZATION

Tables 4-1 and 4-2 summarize the results of risk characterization for this Addendum. In Table 4-1, the refined oral reference dose for DDB, based on the evaluation described in Section 3.0, is used with the same intake assumptions used in the original HRA for the soil ingestion and dermal contact exposure pathways. A DDB soil concentration of 12,660 mg/kg, representing the 95th upper confidence limit of the arithmetic mean concentration for the soil dataset, was conservatively used in these computations. Use of the 95th upper confidence limit of the arithmetic mean concentration is consistent with the RWQCB's request to use the 95th cumulative percentile as a source concentration.

In Table 4-2, the results of the vapor inhalation pathway are presented, again using the same intake assumptions used in the original HRA for dust inhalation exposures. The inhalation reference dose was assumed to be equivalent to the oral reference dose, consistent with the original HRA and Section 3.0 of this Addendum. A separate risk characterization table for revised dust inhalation exposures is not provided, as the revised hazard quotient for this pathway is easily computed based on the ratio of the previous reference dose to the reference dose presented in this evaluation.

In order to evaluate the potential noncarcinogenic health hazard posed by DDB in site soil, and based on the refined toxicity values, the hazard quotients for the four exposure pathways were summed as follows:

Inhalation of dust:	1×10^{-4}
Inhalation of vapors:	3×10^{-7}
Ingestion of soil:	0.07
Dermal contact with soil:	0.41
	0.48

This total hazard quotient, 0.48, is below 1, and therefore indicates that DDB in site soils poses no significant health hazard to potentially exposed workers or other non-residential receptors, as previously concluded in the original HRA.

5 CONCLUSIONS

This Addendum presented revised approaches to establishing toxicity values and fate and transport properties for dodecylbenzene for use in conducting exposure modeling and estimating possible hazards from chemical exposure. A QSAR approach was used in this Addendum, as accepted by and in response to comments received on the original dodecylbenzene health risk assessment prepared in 1994 by the RWQCB.

Using the QSAR approach, fate and transport properties developed for dodecylbenzene were shown to be less conservative than those used in the original health risk assessment. Similarly, the oral reference dose developed to evaluate the toxicity of dodecylbenzene was less conservative than that used in the original health risk assessment. The body of available data on alkylbenzenes therefore indicates that dodecylbenzene is less mobile and less toxic than the conservative values assumed previously using Monsanto data on mixed linear alkylbenzenes.

Results of the SESOIL modeling run using these refined fate and transport parameters, along with physical soil properties measured at the site, indicates that dodecylbenzene is not expected to leach to groundwater over a 99-year period. In fact, the modeling indicates that dodecylbenzene is essentially immobile at the site.

Results of the soil volatilization modeling and other exposure pathways, in combination with the refined reference dose, indicate that possible exposures to dodecylbenzene are below levels of concern to regulatory agencies. Therefore, no further action is required to adequately protect human health or groundwater quality from dodecylbenzene detected in subsurface soils at the site. Based on these results, no deed restriction relative to non-residential use of the site should be necessary.

LIMITATIONS

The services described in this report were performed consistent with generally accepted professional consulting principles and practices. No other warranty, express or implied, is made. These services were performed consistent with our agreement with our client. This report is solely for the use and information of our client unless otherwise noted. Any reliance on this report by a third party is at such party's sole risk.

Opinions and recommendations contained in this report apply to conditions existing when services were performed and are intended only for the client, purposes, locations, time frames, and project parameters indicated. We are not responsible for the impacts of any changes in environmental standards, practices, or regulations subsequent to performance of services. We do not warrant the accuracy of information supplied by others, nor the use of segregated portions of this report.

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TABLES

Table 2-1

Chemical Property Values for Toluene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility[1] (S, mg/L)	Organic soil-water partition coefficient[3] (Koc, log L/kg)	Koc (L/kg)	Henry's Law constant[3] (H, Pa-m3/mol)	H (atm-m3/mol)
520		260		0.0066
515	2.49	309	677	0.0067
470	2.43	269	518	0.0051
570	2.25	178	682	0.0067
347	2.39	245	673	0.0066
530	2.48	302	675	0.0067
500	1.89	78	673	0.0066
627	2.28	191	680	0.0067
546	1.93	85	647	0.0064
550	2.43	269	620	0.0061
595	2.49	309	675	0.0067
538	2.32	209	602	0.0059
515	1.12	13	824	0.0081
470	2.85	708	825	0.0081
354	2.58	380	647	0.0064
479	1.77	59	594	0.0059
573	3.28	1905	519	0.0051
517	2	100	651	0.0064
627	2.18	151	604	0.0060
517	2	100	605	0.0060
517	2.18	151	637	0.0063
520	2.25	178	679	0.0067
534.8	2.18	151	533	0.0053
524	2.26	182	680	0.0067
512	1.99	98	673	0.0066
554			694	0.0068
488				
534				
515				
535				
470				
623				
660				
732				
739				
566				
735				
1548				
581				
507				
542				
530				
715				
585				

Table 2-1 (cont.)

Chemical Property Values for Toluene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility, cont. (mg/L)	Vapor pressure[4] (P, Pa)	P (mmHg)
578		
514		
535		22
507	3800	28.5
520	3792	28.4
534	4000	30.0
555	3826	28.7
580	4000	30.0
524	3749	28.1
561	3881	29.1
428	3560	26.7
578	3786	28.4
530	3792	28.4
529	3800	28.5
272	3786	28.4
575	855	6.4
1581		
515		
265		
461		
707		
580		
538		
525		
440		
525		
515		
530		
535		
545		

Statistical Parameter	S (mg/L)	Koc (L/kg)	H (atm-m3/mol)	P (mmHg)
g. mean			0.01	
SD			0.11	
n			26.00	
Var G mean			0.01	
H95			1.72	
95UCL/G mean			0.01	
H05			-1.66	
5UCL/G mean			0.01	
a. mean	563.63	275.25		26.55
SD	187.54	366.80		6.11
n	74.00	25.00		14.00
+/- 45CL	42.73	143.78		3.20
95UCL	606.36	419.03		29.75
5UCL	520.90	131.46		23.35

mg/L	milligrams per liter
L/kg	liter per kilogram
Pa-m3/mol	pascals-cubic meters per mol
atm-m3/mol	atmospheres-cubic meters per mol
mm Hg	millimeters mercury
g. mean	geometric mean
a. mean	arithmetic mean
SD	standard deviation
n	number of data points in dataset
Var G mean	variance of the geometric mean
H95	statistical lookup value for lognormal distribution
95UCL	95th percentile upper confidence limit of distribution
H05	statistical lookup value for lognormal distribution
5UCL	5th percentile upper confidence limit of distribution
+/- 45CL	45th percentile confidence limit (plus or minus about the mean)

[1] All solubility data from Mackay et al., 1992 except for first (520 mg/L: USEPA, 1995) and second (515 mg/L: Verschueren, 1983) values.

[2] All Koc data from Mackay et al., 1992 except for first value (260 L/kg: USEPA, 1995).

[3] All Henry's Law values from Mackay et al., 1992 except for first value (0.0066 atm-m^3/mol: USEPA, 1995).

[4] All vapor pressure data from Mackay et al., 1992 except for first value (22 mmHg: Verschueren, 1983).

Table 2-2

Chemical Property Values for Ethylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility[1] (S, mg/L)	Organic soil-water partition coefficient[2] (Koc, log L/kg)	Koc (L/kg)	Henry's Law constant[3] (H, Pa-m3/mol)	H (atm-m3/mol)	Vapor pressure[4] (P, Pa)	P (mmHg)
680		220		0.0079		7.00
152	3.04	1096	757	0.0075	1270	9.53
140	1.88	95.50	879	0.0087	1276	9.57
168	2.3	200	854	0.0084	1319	9.89
175	2.21	182	884	0.0087	1297	9.73
208	2.41	257	854	0.0084	1266	9.50
165	2.52	331	800	0.0079	1270	9.53
172	2.47	295	669	0.0066	1270	9.53
159			800	0.0079	1268	9.51
152			689	0.0068	1266	9.50
140			793	0.0079	1280	9.60
112.8			1001	0.0099	283	2.12
177			748	0.0074		
180			864	0.0085		
203			887	0.0088		
151						
153.5						
131						
154						
154						
208						
184						
207						
196						
164						
217						
183						
159						
168						
169						
172						
187						
143						
266						
152						
161						
156						
168						
152						
166						
187						
172						
168						
174						
135						
222						
655						
192						
164						
80.6						
207						
169						
177						
178						
60						
57						
170						
169						
157						

Table 2-2 (cont.)

Chemical Property Values for Ethylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Statistical Parameter	S (mg/L)	Koc (L/kg)	(atm-m3/mol	P (mmHg)
g. mean		256.48		
SD		0.70		
n		8.00		
Var G mean		0.50		
H95		2.90		
95UCL/G mean		711.51		
H05		-1.58		
5UCL/G mean		215.70		
a. mean	183.08		0.01	8.75
SD	97.63		0.00	2.22
n	59.00		15.00	12.00
+/- 45CL	24.91		0.00	1.26
95UCL	207.99		0.01	10.00
5UCL	158.17		0.01	7.49

mg/L	=	milligrams per liter
L/kg	=	liter per kilogram
Pa-m3/mol	=	pascals-cubic meters per mol
atm-m3/mol	=	atmospheres-cubic meters per mol
mm Hg	=	millimeters mercury
g. mean	=	geometric mean
a. mean	=	arithmetic mean
SD	=	standard deviation
n	=	number of data points in dataset
Var G mean	=	variance of the geometric mean
H95	=	statistical lookup value for lognormal distribution
95UCL	=	95th percentile upper confidence limit of distribution
H05	=	statistical lookup value for lognormal distribution
5UCL	=	5th percentile upper confidence limit of distribution
+/- 45CL	=	45th percentile confidence limit (plus or minus about the mean)

[1] All data from Mackay et al., 1992 except for first (680 mg/L, USEPA, 1995) and second (152 mg/L, Verschueren, 1983) values.

[2] All data from Mackay et al., 1992 except for first (220 L/kg, USEPA, 1995) value.

[3] All data from Mackay et al., 1992 except for first (0.0079 atm-m^3/mol) value.

[4] All data from Mackay et al., 1992 except for first (7.00 mmHg, Verschueren, 1983) value.

Table 2-3

Chemical Property Values for Propylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility[1] (mg/L, S)	Log Organic soil-water partition coefficient[2] (log Koc, L/kg)	Koc (L/kg)	Henry's Law constant[3] (H, Pa-m3/mol)	H (atm-m3/mol)	Vapor pressure[4] (P, Pa)	P (mmHg)
60	2.86	724	1109	0.011		2.50
60	2.86	724	1159	0.011	449	3.37
120	2.83	676	700	0.007	457	3.43
55	2.98	955	866	0.009	457	3.43
120	2.86	724	1094	0.011	469	3.52
60			942	0.009	333	2.50
29			1033	0.010	450	3.38
60					449	3.37
54.9						
70						
54.9						
50.1						
87.1						
81.3						
51						
55						
51.9						
55						
57						
93.3						
74.1						
55						
47.1						
52.2						
59.5						
52.1						
45.2						
60						
51.7						
67.6						
46.1						
55						
60.3						
56.1						

Table 2-3 (cont.)

Chemical Property Values for Propylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Statistical Parameter	S (mg/L)	Koc (L/kg)	H (atm-m3/mol)	P (mmHg)
g. mean	59.69	755.09		
SD	0.27	0.13		
n	34.00	5.00		
Var G mean	0.07	0.02		
H95	1.37	2.04		
95UCL/G mean	66.02	873.86		
H05	-1.27	-1.81		
5UCL/G mean	58.31	674.73		
a. mean			0.01	3.19
SD			0.00	0.43
n			7.00	8.00
+/- 45CL			0.00	0.30
95UCL			0.01	3.48
5UCL			0.01	2.89

mg/L	=	milligrams per liter	H95	=	statistical lookup value for lognormal distribution
L/kg	=	liter per kilogram	95UCL	=	95th percentile upper confidence limit of distribution
Pa-m3/mol	=	pascals-cubic meters per mol	H05	=	statistical lookup value for lognormal distribution
atm-m3/mol	=	atmospheres-cubic meters per mol	5UCL	=	5th percentile upper confidence limit of distribution
mm Hg	=	millimeters mercury	+/- 45CL	=	45th percentile confidence limit (plus or minus about the mean)
g. mean	=	geometric mean			
a. mean	=	arithmetic mean			
SD	=	standard deviation			
n	=	number of data points in dataset			
Var G mean	=	variance of the geometric mean			

[1] All data from Mackay et al., 1992 except for first (60 mg/L, Verschueren, 1983) value.
[2] All data from Mackay et al., 1992.
[3] All data from Mackay et al., 1992.
[4] All data from Mackay et al., 1992 except for first (2.50 mmHg; Verschueren, 1983) value.

Table 2-4

Chemical Property Values for Butylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility[1] (mg/L, S)	Log Organic soil-water partition coefficient[2] (log Koc, L/kg)	K_{oc} (L/kg)	Henry's Law constant[3] (H, Pa-m3/mol)	H (atm-m3/mol)	Vapor pressure[4] (P, Pa)	P (mmHg)
12.6	3.39	2455	1300	0.013		1
50.5	3.16	1445	1333	0.013	137	1.03
50.5	3.4	2512			144	1.08
15.4	3.15	1413			137	1.03
17.7	3.32	2089			158	1.19
11.8	3.4	2512			137	1.03
15.4						
13.8						
14.5						
12.2						
13.83						
13.8						
22.8						
12.2						
10.8						
13.8						
13.76						
15						
13.8						
12						

Table 2-4 (cont.)

Chemical Property Values for Butylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Statistical Parameter	S (mg/L)	Koc (L/kg)	H (atm-m3/mol)	P (mmHg)
g. mean	15.89		DI	1.056
SD	0.43		DI	0.062
n	20.00		DI	6.000
Var G mean	0.18		DI	0.004
H95	1.91		DI	1.961
95UCL G mean	20.97		DI	1.117
H05	-1.63		DI	-1.769
5UCL G mean	14.84		DI	1.008
a. mean		2070.96	DI	
SD		521.77	DI	
n		6.00	DI	
+/- 45CL		417.50	DI	
95UCL		2488.46	DI	
5UCL		1653.46	DI	

mg/L = milligrams per liter
L/kg = liter per kilogram
Pa-m3/mol = pascals-cubic meters per mol
atm-m3/mol = atmospheres-cubic meters per mol
mm Hg = millimeters mercury
g. mean = geometric mean
a. mean = arithmetic mean
SD = standard deviation
n = number of data points in dataset
Var G mean = variance of the geometric mean
DI = data insufficient for statistical analysis

H95 = statistical lookup value for lognormal distribution
95UCL = 95th percentile upper confidence limit of distribution
H05 = statistical lookup value for lognormal distribution
5UCL = 5th percentile upper confidence limit of distribution
+/- 45CL = 45th percentile confidence limit (plus or minus about the mea

[1] All data from Mackay et al., 1992.
[2] All data from Mackay et al., 1992.
[3] All data from Mackay et al., 1992.
[4] All data from Mackay et al., 1992 except first (1 mmHg: Verschueren, 1983) value.

Table 2-5

Chemical Property Values for Pentylbenzene[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility (mg/L, S)	Log Organic soil-water partition coefficient (log Koc, L/kg	Koc (L/kg)	Henry's Law constant (H, Pa-m3/mol)	(atm-m3/mol	Vapor pressure (P, Pa)	P (mmHg)
10.5			600	0.0059	43.7	0.328
3.84			617	0.0061	43.7	0.328
3.85					54.9	0.412
3.37						
3.89						

Table 2-5 (cont.)

Chemical Property Values for Pentylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Statistical Parameter	S (mg/L)	Koc (L/kg)	H (atm-m3/mol	P (mmHg)
g. mean	4.59	DI	DI	DI
SD	0.47	DI	DI	DI
n	5.00	DI	DI	DI
Var G mean	0.22	DI	DI	DI
H95	2.95	DI	DI	DI
95UCL/G mea	10.17	DI	DI	DI
H05	-1.59	DI	DI	DI
5UCL/G mean	3.53			
a. mean		DI	DI	DI
SD		DI	DI	DI
n		DI	DI	DI
+/- 45CL		DI	DI	DI
95UCL		DI	DI	DI
5UCL		DI	DI	DI

mg/L	=	milligrams per liter	H95	=	statistical lookup value for lognormal distribution
L/kg	=	liter per kilogram	95UCL	=	95th percentile upper confidence limit of distribution
Pa-m3/mol	=	pascals-cubic meters per mol	H05	=	statistical lookup value for lognormal distribution
atm-m3/mol	=	atmospheres-cubic meters per mol	5UCL	=	5th percentile upper confidence limit of distribution
mm Hg	=	millimeters mercury	+/- 45CL	=	45th percentile confidence limit (plus or minus about the mean)
g. mean	=	geometric mean			
a. mean	=	arithmetic mean			
SD	=	standard deviation			
n	=	number of data points in dataset			
Var G mean	=	variance of the geometric mean			
DI	=	data insufficient for statistical analysis			

[1] All data from Mackay et al., 1992.

Table 2-6

Chemical Property Values for Hexylbenzene[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Water solubility (S, mg/L)	Log Organic soil-water partition coefficient (log Koc, L/kg	Koc (L/kg)	Henry's Law constant (H, Pa-m3/mol)	H (atm-m3/mol	Vapor pressure (P, Pa)	P (mmHg)
1.02			1977	0.020	13.61	0.102
1.02						
0.902						
1.02						
0.971						

Table 2-6 (cont.)

Chemical Property Values for Hexylbenzene
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Statistical Parameter	S (mg/L)	Koc (L/kg)	H (atm-m3/mol)	P (mmHg)
g. mean		DI	DI	DI
SD		DI	DI	DI
n		DI	DI	DI
Var G mean		DI	DI	DI
H95		DI	DI	DI
95UCL/G mean		DI	DI	DI
H05		DI	DI	DI
5UCL/G mean				
a. mean	0.99	DI	DI	DI
SD	0.05	DI	DI	DI
n	5.00	DI	DI	DI
+/- 45CL	0.05	DI	DI	DI
95UCL	1.03	DI	DI	DI
5UCL	0.94	DI	DI	DI

mg/L	=	milligrams per liter	H95	=	statistical lookup value for lognormal distribution
L/kg	=	liter per kilogram	95UCL	=	95th percentile upper confidence limit of distribution
Pa-m3/mol	=	pascals-cubic meters per mol	H05	=	statistical lookup value for lognormal distribution
atm-m3/mol	=	atmospheres-cubic meters per mol	5UCL	=	5th percentile upper confidence limit of distribution
mm Hg	=	millimeters mercury	+/- 45CL	=	45th percentile confidence limit (plus or minus about the mean)
g. mean	=	geometric mean			
a. mean	=	arithmetic mean			
SD	=	standard deviation			
n	=	number of data points in dataset			
Var G mean	=	variance of the geometric mean			
DI	=	data insufficient for statistical analysis			

[1] All data from Mackay et al., 1992.

Table 2-7

Results of Statistical Distribution Tests[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Parameter	Normal distribution critical value [2]	Lognormal distribution critical value [3]	W-Test Look-up value	D-Test Range for λ	Closest to normal ?[4]	Closest to lognormal ?[4]
Toluene						
solubility	-29.5	38,939	-	-2.64 to 1.20	yes	-
partition coefficient	0.829	0.94[5]	0.918	-	-	-
Henry constant	0.885	0.894	0.918	-	-	yes
vapor pressure	0.426	0.37	0.866	-	yes	-
Ethylbenzene						
solubility	-27	9,970	-	-2.72 to 1.09	yes	-
partition coefficient	0.685	0.934	0.803	-	-	-
Henry constant	0.947	-	0.874	-	-	-
vapor pressure	0.392	0.369	0.850	-	yes	-
Propylbenzene						
solubility	0.787	0.883	0.931	-	-	yes
partition coefficient	0.703	0.726	0.762	-	-	yes
Henry constant	0.848	-	0.803	-	-	-
vapor pressure	0.596	0.576	0.803	-	yes	-
Butylbenzene						
solubility	0.525	0.660	0.905	-	-	yes
partition coefficient	0.792	-	0.788	-	-	-
Henry constant	ID	ID	-	-	-	-
vapor pressure	0.735	0.740	0.762	-	-	yes
Pentylbenzene						
solubility	0.614	0.661	0.762	-	-	yes
partition coefficient	ID	ID	-	-	-	-
Henry constant	ID	ID	-	-	-	-
vapor pressure	ID	ID	-	-	-	-
Hexylbenzene						
solubility	0.758	0.754	0.762	-	yes	-
partition coefficient	ID	ID	-	-	-	-
Henry constant	ID	ID	-	-	-	-
vapor pressure	ID	ID	-	-	-	-
Heptylbenzene						
solubility	ID	ID	-	-	-	-
partition coefficient	ID	ID	-	-	-	-
Henry constant	ID	ID	-	-	-	-
vapor pressure	ID	ID	-	-	-	-
Octylbenzene						
solubility	ID	ID	-	-	-	-
partition coefficient	ID	ID	-	-	-	-
Henry constant	ID	ID	-	-	-	-
vapor pressure	ID	ID	-	-	-	-

ID = insufficient data for statistical analysis

Bolded values signify distribution determination.

[1] Shapiro-Wilk Test used for data sets with ≤ 50 values; D'Agostino's Test used for data sets with > 50 values.

[2] If the critical value as calculated by the W-Test (or D-Test as appropriate) is higher than the look up value (or is inside the λ range), the data is considered to be normal. If the data is not found to be normally distributed, the data set is transformed logarithmically and recalculated.

[3] If the lognormal critical value is higher than the look up value, (or inside the λ range), the data is considered to be lognormally distributed.

[4] If the data set was found to be neither normal or lognormal, the critical value closest to the look up value (or Y range) was noted and this distribution was assumed.

[5] Critical value indicates the data set to be lognormally distributed; however a normal distribution was assumed for this evaluation (see text, Section 2.1.2).

Table 2-8

Regression Analysis for Solubility and Vapor Pressure
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

SOLUBILITY (S, mg/L)	Number of methylene units	5LCL	95UCL	log mean	log 5LCL	log 95UCL
Toluene	0	520.36	621.77	2.76	2.716	2.794
Ethylbenzene	1	158.17	207.99	2.26	2.199	2.318
Propylbenzene	2	58.31	66.02	1.78	1.766	1.820
Butylbenzene	3	14.84	20.97	1.20	1.172	1.322
Pentylbenzene	4	3.53	10.17	0.66	0.548	1.007
Hexylbenzene	5	0.94	1.03	-0.01	-0.026	0.014
VAPOR PRESSURE (P, mmHg)						
Toluene	0	23.35	29.75	1.42	1.368	1.474
Ethylbenzene	1	7.49	10.00	0.94	0.875	1.000
Propylbenzene	2	2.89	3.48	0.50	0.461	0.542
Butylbenzene	3	1.01	1.12	0.02	0.003	0.048

SOLUBILITY (S, mg/L)	Slope	intercept	r^2	log S (DDB)	S (DDB)
mean	-0.5483	2.813	0.9970549	-3.22	0.0006
5LCL	-0.5504	2.772	0.9966555	-3.28	0.0005
95UCL	-0.5237	2.855	0.9763441	-2.91	0.0012
VAPOR PRESSURE (P, mmHg)					
				log P (DDB)	P (DDB)
mean	-0.4640	1.419	0.9996723	-3.68	0.00021
5LCL	-0.4509	1.353	0.9989324	-3.61	0.00025
95UCL	-0.4735	1.476	0.9997976	-3.73	0.00019

DDB = dodecylbenzene
mg/L = milligrams per liter
mm Hg = millimeters mercury
5LCL = 5th percentile lower confidence limit
95UCL = 95th percentile upper confidence limit
r^2 = regression coefficient

Table 2-9

Calculation of Dodecylbenzene Henry's Law Constant[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

	Vapor pressure[2] (mmHg)	Vapor pressure (atm)	Water solubility[3] (mg/L)	Water solubility[4] (g/m3)	MW (g/mole)	Water solubility[5] (mol/m3)	Henry Constant[6] (atm-m3/mol)
Mean	0.00021	2.72E-07	0.0006	0.0006	246.4	2.45E-06	0.11
5/95 CL (low value)	0.00019	2.44E-07	0.0012	0.0012	246.4	5.04E-06	0.05
5/95 CL (high value)	0.00025	3.26E-07	0.0005	0.0005	246.4	2.12E-06	0.15

mm Hg = millimeters mercury
atm = atmospheres
mg/L = milligrams per liter
UCF = unit conversion factor
g/mg = grams per milligram
L/m^3 = liters per cubic meter
g/m3 = grams per cubic meter
MW = molecular weight (of DDB)
g/mole = grams per mole
mol/m3 = moles per cubic meter
atm-m3/mol = atmospheres-cubic meters per mole
5/95 CL (low value) = 5th or 95th percentile confidence limit (see Table 2-8)
5/95 CL (high value) = 5th or 95th percentile confidence limit (see Table 2-8)

[1] Based on regression analysis results (Table 2-8).
[2] Table 2-8.
[3] Table 2-8.
[4] Solubility (mg/L) x 0.001 g/mg x 1,000 L/m^3.
[5] Solubility (g/m^3)/ MW.
[6] Vapor pressure (atm)/ solubility (mol/m^3).

Table 2-10

Calculation of Dodecylbenzene Organic Soil-Water Partition Coefficient[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

	Water solubility[2] (mol/m3)	Water density (g/cm^3)	MW (g/mol)	Water solubility[3] (mol fraction)	Water solubility[4] (log mol fraction)	Log partition coefficient[5] (log cm^3/g)	Partition coefficient[6] (cm^3/g – L/kg)
Mean	2.45E-06	1	18	4.42E-11	-10.35	6.03	1.1E+06
5 LCL	5.04E-06	1	18	9.08E-11	-10.04	5.86	7.3E+05
95 UCL	2.12E-06	1	18	3.81E-11	-10.42	6.07	1.2E+06

mol/m3 = moles per cubic meter
UCF = unit conversion factor
g/cm^3 = grams per cubic centimeter
MW = molecular weight (of water)
g/mole = grams per mole
L/kg = liters per kilogram
5LCL = 5th percentile lower confidence limit (see Table 2-8)
95UCL = 95th percentile upper confidence limit (see Table 2-8)

[1] Based on regression analysis results for solubility (Table 2-8) and regression relationship for the partition coefficient (Lyman et al., 1990; Cal-EPA, 1986).
[2] Table 2-9.
[3] Solubility (mol/m^3) x 1E-06 m3/cm3 x water density x MW (water).
[4] Log solubility (mole fraction).
[5] 0.44 - 0.54 x solubility (log mole fraction) (Lyman et al., 1990; Cal-EPA, 1986).
[6] $10^{\text{log partition coefficient}}$.

Table 2-11

Calculation of Dodecylbenzene Air Diffusion Coefficient with Fuller's Method[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Parameter definition	Units	Symbol	Value
Absolute Temperature	Degrees K	T	293
Molecular Weight of Compound	g/mol	MWi	246.44
Molecular Weight of Air	g/mol	MWa	28.8
Absolute Pressure	atm	Pa	1
Molecular Diffusion Volume of Air	cm3/mol	Va	20.1
Diffusion Volume of Carbon	cm3/mol	Vc	16.5
Diffusion Volume of Chlorine	cm3/mol	Vcl	19.5
Diffusion Volume of Hydrogen	cm3/mol	Vh	1.98
Diffusion Volume of Fluorine	cm3/mol	Vf	25
Diffusion Volume of Oxygen	cm3/mol	Vo	5.48
Diffusion Volume of Aromatic Ring	cm3/mol	Var	-20.2
Diffusion Volume of Sulfur	cm3/mol	Vs	17
Diffusion Volume of Nitrogen	cm3/mol	Vn	5.69
Diffusion Volume of Bromine	cm3/mol	Vb	35
Diffusion Volume of Heterocyclic Ring	cm3/mol	Vhr	-20.2
Number of C atoms	--	Nc	18
Number of Cl atoms	--	Ncl	0
Number of H atoms	--	Nh	30
Number of F atoms	--	Nf	0
Number of O atoms	--	No	0
Number of Aromatic rings	--	Nar	1
Number of S atoms	--	Ns	0
Number of N atoms	--	Nn	0
Number of Br atoms	--	Nb	0
Number of Heterocyclic rings	--	Nhr	0
Molecular Diffusion Volume of Compound[2]	cm3/mol	Vi	336.2
Diffusion Coefficient[3]	cm^2/sec	Di	4.37E-02

[1] Model from USEPA, 1988.
[2] NcVc + NclVcl + NhVh + NfVf + NoVo + NarVar + NsVs + NnVn + NbVb + NhrVhr
[3] $((0.001T^{1.75})(1/MWi + 1/MWa)^{0.5})/(PaVi^{.33} + Va^{.33})^2)$

Table 2-12

Estimation of Volatile Emissions from Saturating Concentrations of Dodecylbenzene[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Parameter definition	Units	Symbol	Value
Mole fraction of component approximated as weight fraction [2]	--	xi	0.01266
Vapor pressure of pure component [3]	mm Hg	p	0.00021
Partial pressure of component i in mixture[4]	mm Hg	pi	2.659E-06
Gas phase concentration of component i above mixture[5]	mol/L	Csg	1.456E-10
Universal gas constant	m Hg-L/mol-deg	R	62.32
Temperature	degrees K	T	293
Gas phase concentration of component i above mixture[6]	mg/m^3	Csg'	0.0
Molecular weight of component i	g/mol	M	246
Conversion factor	$mg\text{-}L/g\text{-}m^3$	CF	1.00E+06
Air diffusion coefficient[7]	cm^2/sec	Di	0.044
Air diffusion coefficient[8]	m2/sec	Di'	0.0000044
Conversion factor	m^2/cm^2	CF'	0.0001
Total soil porosity[9]	--	Pt	0.290
Height of clean soil cover [10]	m	L	0.762
Height of clean soil cover [11]	ft	L	2.5
Conversion factor	m/ft	CF"	0.3048
Vapor flux of component i at soil surface [12]	$mg/sec\text{-}m^2$	F	3.972E-08

mol/L = moles per liter
degrees K (or "degK") = degrees kelvin
mg = milligrams
ft = feet

For other abbreviations, see Tables 2-1 through 2-11

[1]Calculation based on Raoult's Law and Shen's model (Shen, 1981 as recommended in USEPA, 1988).
[2]Based on 12,660 mg/kg soil concentration (95UCL/ a. mean).
[3]Vapor pressure from Table 2-8.
[4]xip.
[5]pi/RT.
[6]CsgMCF
[7]Table 2-11.
[8]DiCF'.
[9]Measured site value.
[10]LCF".
[11]Based on available site data (EMCON, 1992,1993a,b) which show detectable concentrations no shallower than about 5 feet bgs.
[12]Calculated using the equation Csg'Di'Pt^1.333/L.

Table 2-13

Outdoor Air Concentration of Dodecylbenzene[1]
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Parameter definition	Units	Symbol	Value
Vapor flux of NAPL component at soil surface[2]	$mg/sec\text{-}m^2$	F	3.97E-08
Mean annual wind speed[3]	m/sec	u	2.4
Effective mixing height[3]	m	H	2
Crosswind width of box[3]	m	w	18
On-site DDB vapor outdoor air concentration[4]	mg/m^3	Ca	1.49E-07

[1] Box model from Cal-EPA, 1994 and USEPA, 1991.
[2] From Table 2-12.
[3] Same parameter values as used in original HRA for dust inhalation (EMCON, 1994).
[4] (F x w)/(H x u)

Table 3-1

Relevant Toxicity Data for Alkylbenzenes
Dodecylbenzene Risk Assessment
Dial Main Facility
Commerce, California

Chemical	Test Species	Exposure Route	Exposure Duration	NOAEL[1] (mg/kg/day)	Endpoint[2]	LOAEL[3] (mg/kg/day)	LD50[4] (mg/kg)	Source[5]
Benzene	rat	oral	acute	NA	death	NA	930-3400	1,2
	rat	oral	6 months	1	leukopenia	10	NA	3
Toluene	rat	gavage	acute	NA	death	NA	2600-7300	4
	mouse	oral	single dose	1800-2350	developmental	NA	NA	5,6
	mouse	oral	single dose	1800-2350	reproduction	NA	NA	6
	rat	oral	6mo; 5d/wk	590	hepatic/renal/hemato	NA	NA	3
	mouse	water	42 days	19.7	behavioral/neuro	98.3	NA	7
Ethylbenzene	rat	gavage	182d; 5d/wk	97.1	hepato/renal	291	NA	3
	rat	oral	acute	NA	death	NA	3500-5460	3,8
Propylbenzene	rat	oral	acute	NA	death	NA	6040	9
Butylbenzene	rat	oral	acute	NA	death	NA	5000 (LDLo)	9
Alkylate 215[4]	rat	oral	acute	NA	death	NA	17000	10
(C10 - C13 mixture)	rat	oral	subchronic	5	repro effects	50	NA	10

NA Not applicable.

[1] No-Observed Adverse Effect Level reported by authors.

[2] Target toxic endpoint evaluated by authors.

[3] Lowest-Observed Adverse Effect Level reported by authors.

[4] Mixture represents 21.43% C10, 42.6 % C11, 35% C12, 0.74% C13 (Robinson and Schroeder 1992).

[5] References as follows:
1 = ATSDR 1987
2 = Lewis 1992
3 = Wolf et al. 1956 as cited in ATSDR 1987
4 = ATSDR 1989
5 = Seidenberg et al. 1986 as cited in ATSDR 1989
6 = Smith 1983 as cited in ATSDR 1989
7 = Kostas and Hotchin 1981 as cited in ATSDR 1989
8 = Smyth et al. 1962 as cited in USEPA 1987
9 = RTECS 1996
10 = Monsanto 1993

Table 3-2

Derivation of Dodecylbenzene Reference Dose
Dodecylbenzene Risk Assessment
Dial Main Facility
Commerce, California

Parameter	Acronym	Value	Units	Basis	Source
LD50	LD50	18,500	mg/kg/day	regression equation	Table 3-1; Figure 3-1
Extrapolation factor	UF	$5x10^{-6}$	unitless	LD50 to chronic NOAEL	Layton et al., 1987
Oral reference dose	RfDo	0.09	mg/kg/day	LD50 x UF	Layton et al., 1987

LD50 Lethal dose to 50 percent of tested animals.

NOAEL No-observed adverse effects level.

See text Section 3.4 for explanation.

Table 4-1

Risk Characterization for Soil Ingestion and Dermal Contact Exposures
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Soil Ingestion

Parameter	Units	Symbol	Value
ADD for soil ingestion[1]	mg/kg-day	ADDsi	0.006
On-site worker soil ingestion rate[2]	mg/day	IR	50
Exposure frequency[2]	days/year	EF	250
Exposure duration[2]	years	ED	25
Body weight[2]	kg	BW	70
Averaging time[3]	days	AT	9125
DDB soil concentration[2]	mg/kg	Cs	12,660
Unit conversion factor	kg/mg	CF	1.00E-06
Chronic oral reference dose for DDB[4]	mg/kg-day	RfDco	0.09
Soil ingestion hazard quotient[5]	--	HQsi	0.07

Dermal Soil Contact

Parameter	Units	Symbol	Value
ADD for dermal soil contact[6]	mg/kg-day	ADDd	0.037
On-site worker exposed skin surface area[2]	mg/day	SA	2980
Soil to skin adherence rate[2]	mg/cm^2-event	AR	1
Absorption factor[2]	--	Ab	0.1
Exposure frequency[2]	days/year	EF	250
Exposure duration[2]	years	ED	25
Body weight[2]	kg	BW	70
Averaging time[3]	days	AT	9125
DDB soil concentration[2]	mg/kg	Cs	12,660
Unit conversion factor	kg/mg	CF	1.00E-06
Chronic oral reference dose for DDB[4]	mg/kg-day	RfDco	0.09
~~Soil ingestion~~ hazard quotient[7]	--	HQd	0.41

Dermal soil contact

[1] (Cs x CF x IR x EF x ED)/(BW x AT)
[2] Same parameter values as for original HRA (EMCON, 1994).
[3] ED x 365 days/year
[4] From Table 3-2
[5] ADDsi/RfDco
[6] (SA x AR x Ab x EF x ED x Cs x CF)/(BW x AT)
[7] ADDd/RfDco

Table 4-2

Risk Characterization for Vapor Inhalation Exposures
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

Parameter	Units	Symbol	Value
ADD for outdoor vapor inhalation[1]	mg/kg-day	ADDvi	3E-08
On-site worker Inhalation rate[2]	m^3/day	IR	20
Exposure frequency[2]	days/year	EF	250
Exposure duration[2]	years	ED	25
Body weight[2]	kg	BW	70
Averaging time[3]	days	AT	9125
Chronic inhalation reference dose for DDB[4]	mg/kg-day	RfDci	0.09
Outdoor vapor inhalation hazard quotient[5]	--	HQvi	3E-07

[1] (Ca [from Table 2-13]x IR x EF x ED)/(BW x AT)

[2] Same parameter values as for original HRA (for dust inhalation; EMCON, 1994).

[3] ED x 365 days/year

[4] From Table 3-2

[5] ADDvi/RfDci

FIGURES

Figure 1-1

Conceptual Site Model
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

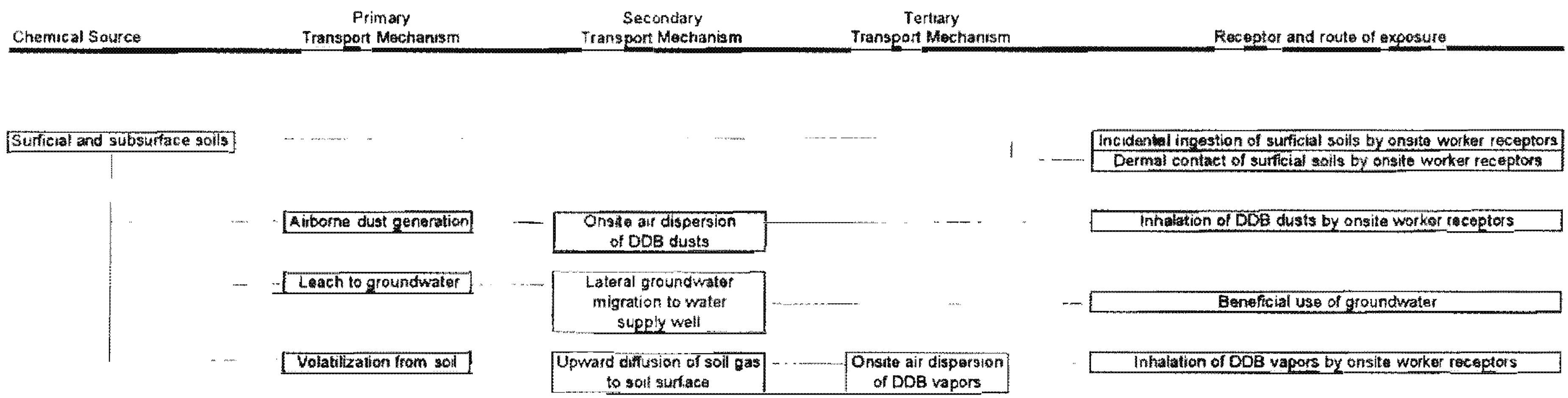


Figure 2-1

Structure-Solubility Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

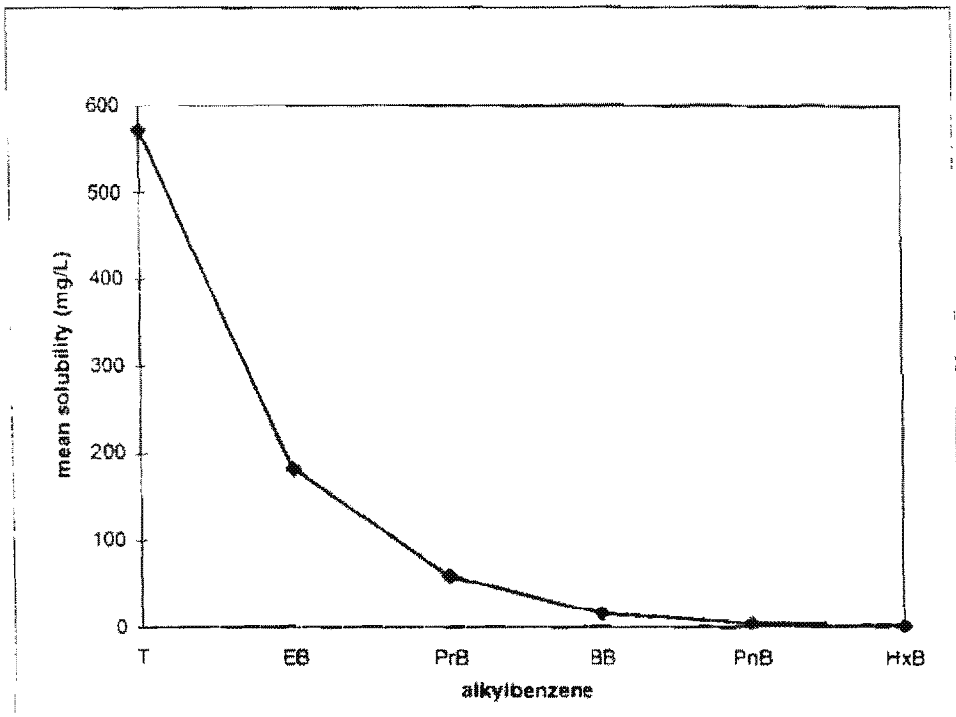


Figure 2-2

Structure-Vapor Pressure Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

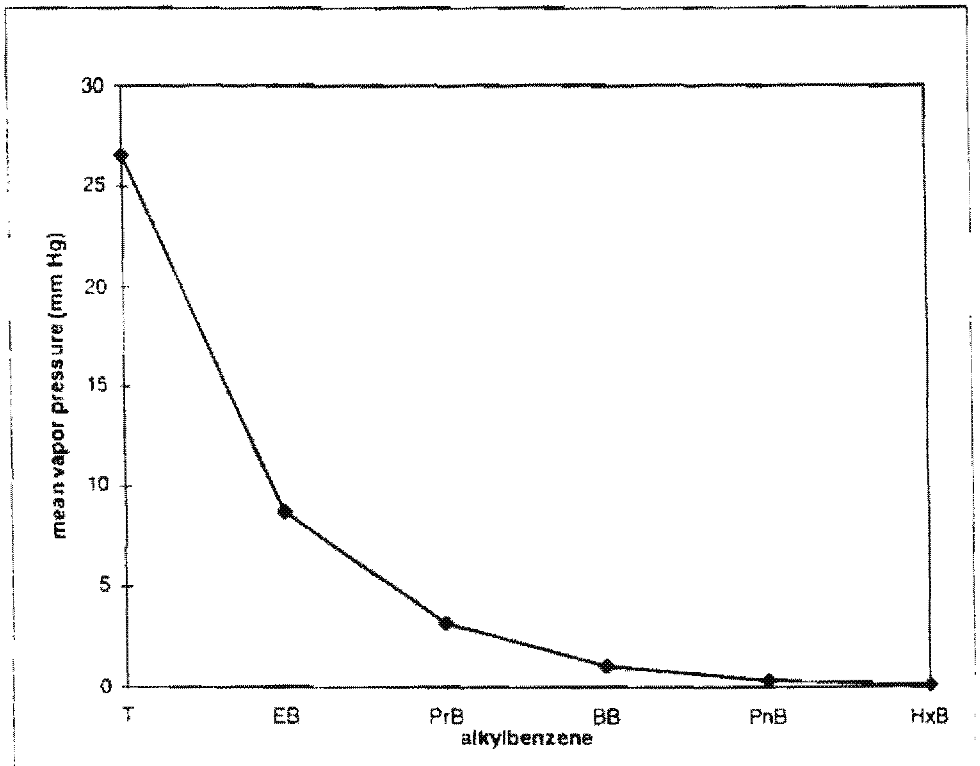


Figure 2-3

Structure-Koc Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

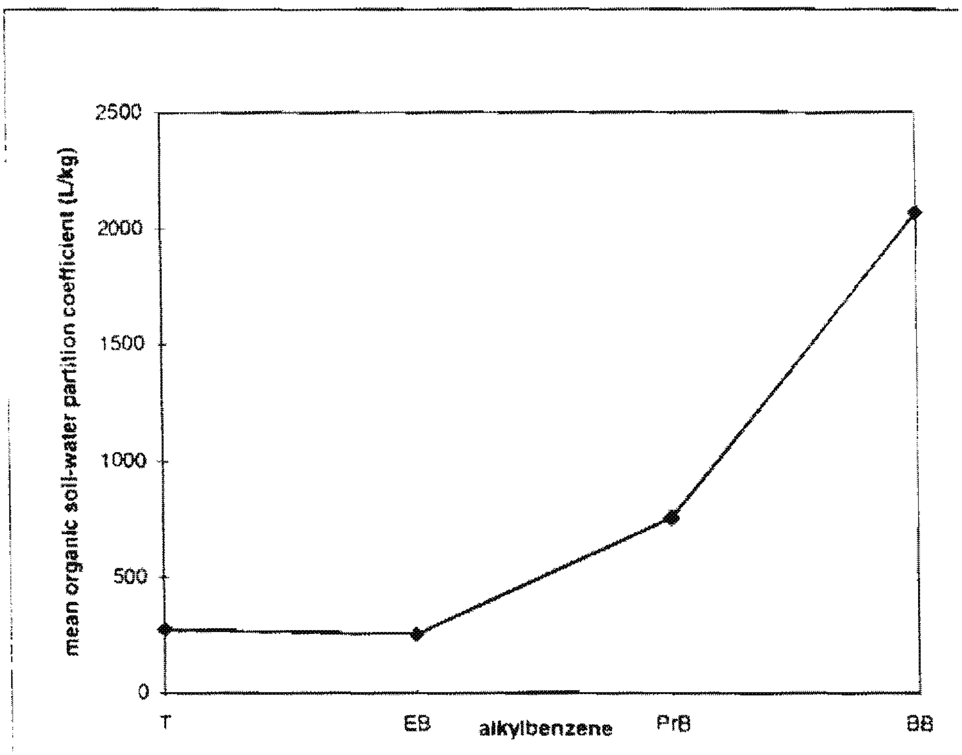


Figure 2-4

Structure-Henry Constant Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

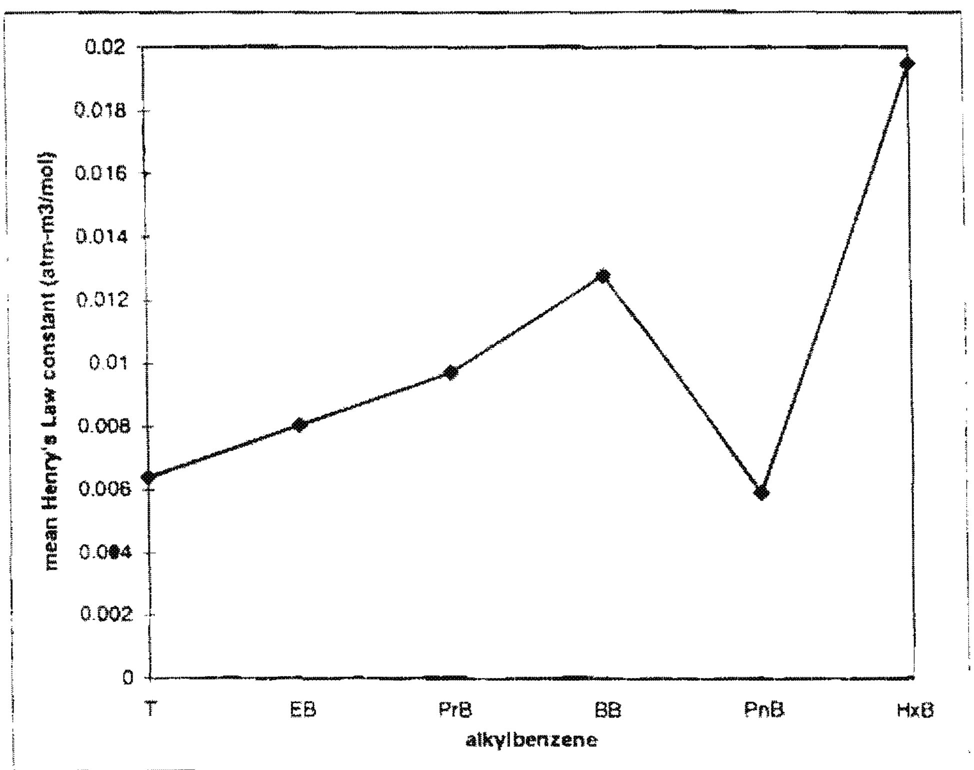


Figure 2-5

Log of Structure-Solubility Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

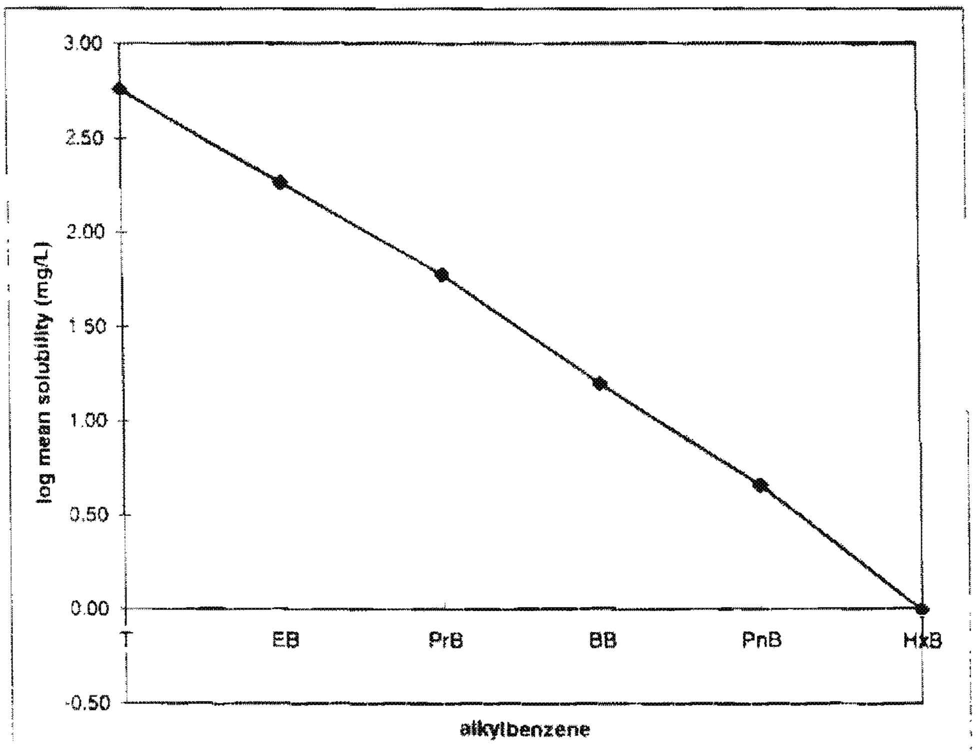


Figure 2-6

Log of Structure-Vapor Pressure Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

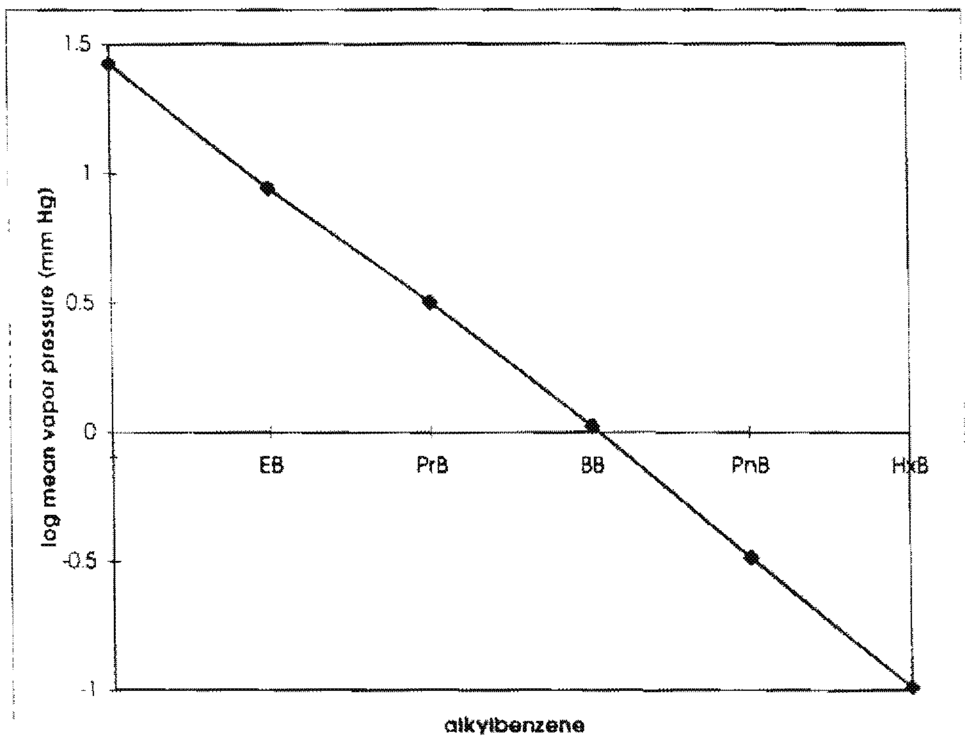


Figure 2-7

Log of Structure-Koc Relationship for the Linear Alkylbenzenes
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California

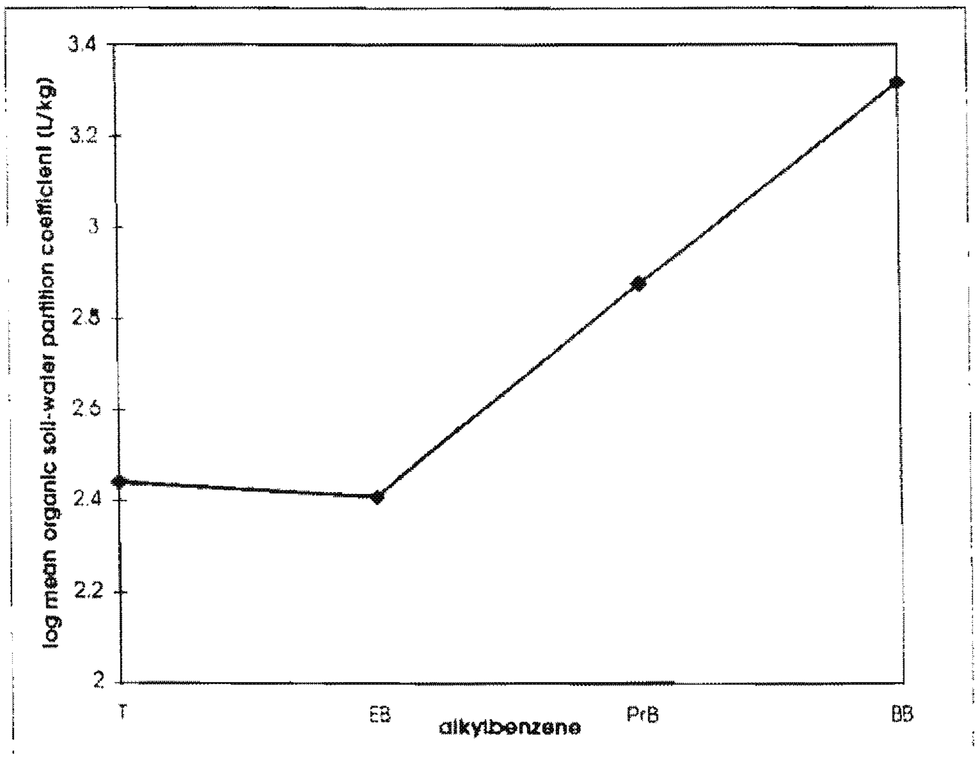
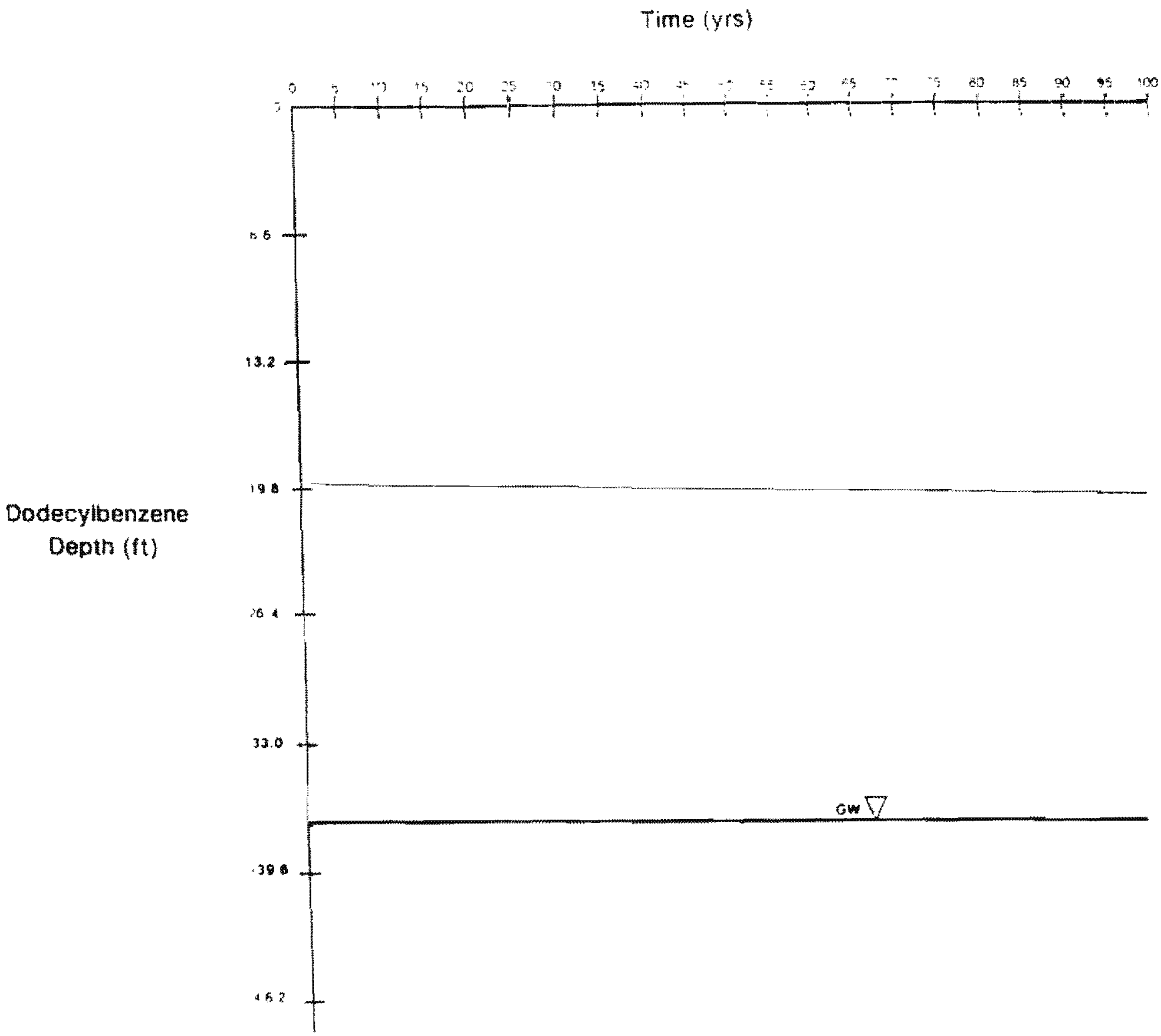


Figure 2-8

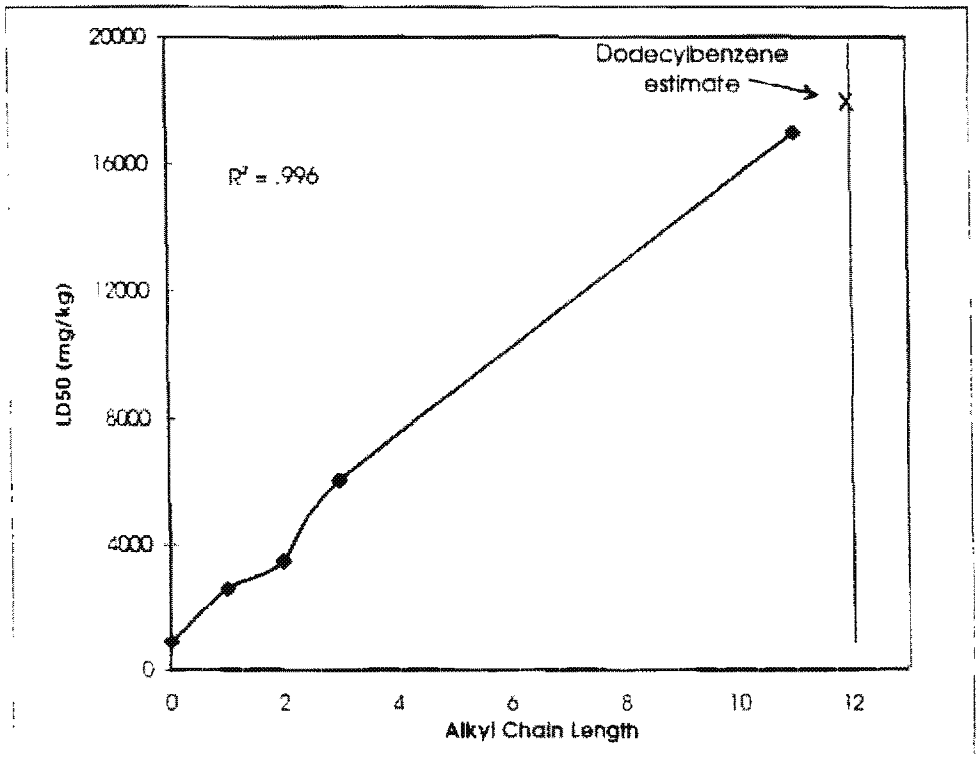
SESOIL Results
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California



H:\SAC\CKF\EXCELDAT\SESOIL.XLS

Figure 3-1

Relationship of Alkyl Chain Length and Oral LD50 Values
Dodecylbenzene Health Risk Assessment Addendum
Dial Corporation Main Facility
2300 Rayo Avenue
South Gate, California



APPENDIX A

SOIL BORING LOGS

November 1996
Project No. 96-48-3411

LOCATION: Alkyate loading sump area
SURFACE EL: Not Surveyed

DEPTH, ft	SAMPLE NO.	SAMPLER BLOWCOUNT	MATERIAL DESCRIPTION	PID READING	TOTAL ORGANIC CARBON, mg/kg	UNIT DRY WEIGHT, pcf	WATER CONTENT, %	POROSITY, %	PERMEABILITY, cm/sec
0–8			**ARTIFICIAL FILL (af)** SAND (SP): brown to dark brown, moist, with gravel (concrete debris), wood fragments, no odor						
5	EB2-5	(20)		0					
8–13			**ALLUVIUM (Qal)** Silty SAND (SM): loose, brown to dark brown, very moist, no odor, dark brown staining						
10	EB2-10	(19)		5.7					1.16E-06
13–20			Sandy CLAY (CL): very stiff, dark brown to brown, very moist, no odor or staining						
15	EB2-15	(12)		0					
20	EB2-20	(25)	Silty fine SAND (SM): dark brown to brown, very moist, no odor or staining	0	0.31	90	31	47	
23–26			Sandy CLAY (CL): very stiff, light brown to brown, no odor or staining						
25	EB2-25	(23)		1.2	0.33	86	35	49	1.79E-07
26–28			Silty fine SAND (SM): dense, dark brown to brown, very moist, no odor or staining						
28–31			Sandy CLAY (CL): stiff, light brown to brown, very moist, no odor or staining						
30	EB2-30	(26)		1.3					
31–41.5			Silty fine SAND (SM): dense, brown to light brown, very moist, no odor or staining						
35	EB2-35	(29)		1		90	23	46	
39			- wet below 39'						
40	EB2-40	(80)		1.5					

COMPLETION DEPTH: 41-1/2 ft
DEPTH TO WATER:
First Encountered (▽): 39.0 ft
At End of Drilling (▼): ft
BACKFILLED WITH: Bentonite/Native
DRILLING DATE: September 20, 1996

DRILLING METHOD: Hollow Stem Auger
DRILLED BY: Valley Well Drilling
LOGGED BY: JRCook
CHECKED BY: MFlack

The log and data presented are a simplification of actual conditions encountered at the time of drilling at the drilled location. Subsurface conditions may differ at other locations and with the passage of time.

LOG OF DRILL HOLE NO. EB- 2
Dial Corporation

63411GV (63411/EB- 2)
11/18/96\12:58

LOCATION: Alkylate loading sump area

SURFACE EL: Not Surveyed

ELEVATION, ft	DEPTH, ft	MATERIAL SYMBOL	SAMPLE NO.	SAMPLERS	SAMPLER BLOWCOUNT	MATERIAL DESCRIPTION	PID READING	TOTAL ORGANIC CARBON, mg/kg	UNIT DRY WEIGHT, pcf	WATER CONTENT, %	POROSITY, %	PERMEABILITY, cm/sec
	2					**ARTIFICIAL FILL (af)** Silty fine SAND (SM): brown to dark brown, moist, metal, wire and wood fragments, no odor, dark brown staining						
	4											
	6		EB3-5		(26)		14.8					
	8					**ALLUVIUM (Qal)** Silty SAND (SM): loose, brown to dark brown, very moist, no odor, with dark brown staining						
	10		EB3-10		(9)		1.2					
	12											
	14											
	16		EB3-15		(23)		4.6	0.34				
	18											
	20		EB3-20		(23)		3.1		93	28	45	
	22											
	24					Sandy CLAY (CL): stiff, brown to light brown, very moist, no odor or staining						
	26		EB3-25		(15)		3.7		87	34	49	1.87E-07
	28											
	30		EB3-30		(26)		5.9					
	32					Silty fine SAND (SM): dense, brown to light brown, very moist, no odor or staining						
	34											
	36		EB3-35		(45)		5.8	0.25				
	38											
	40		EB3-40		(70)		5.7					
	42											
	44											
	46											
	48											

COMPLETION DEPTH: 41-1/2 ft
DEPTH TO WATER:
First Encountered (▽): 37.0 ft
At End of Drilling (▼): 37.0 ft
BACKFILLED WITH: Bentonite/Native
DRILLING DATE: September 20, 1996

DRILLING METHOD: Hollow Stem Auger
DRILLED BY: Valley Well Drilling
LOGGED BY: JRCook
CHECKED BY: MFlack

The log and data presented are a simplification of actual conditions encountered at the time of drilling at the drilled location. Subsurface conditions may differ at other locations and with the passage of time.

LOG OF DRILL HOLE NO. EB- 3
Dial Corporation

LOCATION: The drill hole location referencing local landmarks or coordinates
SURFACE EL: Using local, MSL, MLLW or other datum

ELEVATION, ft	DEPTH, ft	SAMPLE NO.	BLOWCOUNT / REC"/DRIVE"	MATERIAL DESCRIPTION	
-12	2	1	25	Well graded GRAVEL (GW)	COARSE GRAINED
-14	4	2	(25)	Poorly graded GRAVEL (GP)	COARSE GRAINED
-16	6			Well graded SAND (SW)	COARSE GRAINED
-18	8	3	(25)	Poorly graded SAND (SP)	COARSE GRAINED
-20	10	4	(25)	Clayey SAND (SC)	COARSE GRAINED
-22	12	5	18"/30"	Silty SAND (SM)	COARSE GRAINED
-24	14	6		SAND with silt (SP-SM)	COARSE GRAINED
-26	16			Fat CLAY (CH)	FINE GRAINED
-28	18	7		Lean CLAY (CL)	FINE GRAINED
-30	20	8	20"/24"	Silty CLAY (CL-ML)	FINE GRAINED
-32	22	9	(25)	Elastic SILT (MH)	FINE GRAINED
-34	24	10	30"/30"	SILT (ML)	FINE GRAINED
-36	26			Clayey SILT (ML/CL)	FINE GRAINED
-38	28	11	20"/24"	SANDSTONE	ROCK
-40	30			SILTSTONE	ROCK
-42	32			CLAYSTONE	ROCK
-44	34			MUDSTONE	ROCK
-46	36			GRANITE	ROCK
-48	38			SHALE	ROCK
				Paving and/or Base Materials	

General Notes

1. Soil Texture Symbol
2. Sloped line in symbol column indicates transitional boundary
3. Samplers and sampler dimensions (unless otherwise noted in report text) are as follows:

   Symbol for:
   1. SPT Sampler, driven 1 3/8" ID, 2" OD
   2. CA Liner Sampler, driven 2 3/8" ID, 3" OD
   3. CA Liner Sampler, disturbed 2 3/8" ID, 3" OD
   4. Recovery Interval
   5. Thin-walled Tube, pushed 2 7/8" ID, 3" OD
   6. Bulk Bag Sample (from cuttings)
   7. Hand Auger Sample
   8. Rock Core Sample
   9. No Sample Recovered
   10. Vibracore Sample
   11. Pitcher Sample
4. Sampler Driving Resistance

   Number of blows with 140 lb. hammer, falling 30-in. to drive sampler 1-ft. after seating sampler 6-in.; for example,

Blows/ft	Description
25	25 blows drove sampler 12" after initial 6" of seating
86/11"	After driving sampler the initial 6" of seating, 36 blows drove sampler through the second 6" interval, and 50 blows drove the sampler 5" into the third interval
50/6"	50 blows drove sampler 6" after initial 6" of seating
Ref/3"	50 blows drove sampler 3" during initial 6" seating interval
5. Blow counts for California Liner Sampler shown in ( )
6. Length of sample symbol approximates recovery length
7. Classification of Soils per ASTM D2487 or D2488
8. Geologic Formation noted in bold font at the top of interpreted interval
9. Strength Legend

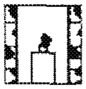
   Q = Unconfined Compression
   u = Unconsolidated Undrained Triaxial
   t = Torvane
   p = Pocket Penetrometer
   m = Miniature Vane
10. Water Level Symbols

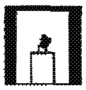
    ▽ Initial or perched water level
    ▼ Final ground water level
    Seepages encountered
11. Rock Quality Designation (RQD) is the sum of recovered core pieces greater than 4 inches divided by the length of the cored interval

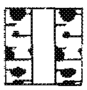
KEY TO TERMS & SYMBOLS USED ON LOGS

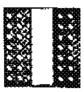
Well Construction Diagram

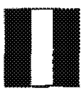

Well Cap

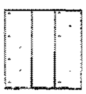

Protective concrete cover

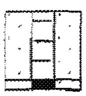

Aboveground cover

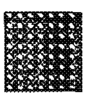

Concrete

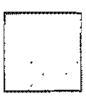

Grout/neat cement

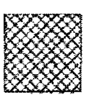

Bentonite pellets


Sand


Slotted pipe w/bottom cap


Grout plug


Sand Backfill


Native Backfill

A. The different types of well constructed include but are not limited to monitoring, vapor extraction, and piezometer.

B. Types and sizes of the materials used are as described in report text

General Notes, continued

12 Refer to report text for EPA Test Methods used

13 Commonly used acronyms:

MSL	Mean Sea Level
MLLW	Mean Lower Low Water
EL	Elevation
FT	Foot or Feet
IN	Inch or Inches
KSF	Kips Per Square Foot
TSF	Tons Per Square Foot
PCF	Pounds Per Cubic Foot
Su	Undrained Shear Strength
MG/KG	Milligrams Per Kilograms
UG/KG	Micrograms Per Kilograms
PPM	Parts Per Million
ND	Not Detected
D	Detected
NA	Not Analyzed
--	Not Analyzed
PID	Photoionization Detector
MTBE	Methyl Tertiary Butyl Ether
TPH	Total Petroleum Hydrocarbons
PCE	Tetrachloroethylene
TCE	Trichloroethene
EDC	1,2-Dichloroethane
cis-1,2-DCE	cis-1,2-dichloroethane
SVOC	Semi-Volatile Organic Compounds

14 PID READING measured in parts per million by volume (ppmv)

15 Kelly Bar Weights used with bucket auger drill rig.

0 - 30 ft	3450 lbs
30 - 60 ft	2050 lbs
60 - 90 ft	1140 lbs

KEY TO TERMS & SYMBOLS USED ON LOGS con't

MOISTURE AND DENSITY DETERMINATIONS

Job No: 96-48-3411	Job Name: DIAL CORP	Date:	10/2/96
Client:	CITY OF CAMARILLO		
Unit Weight of Water (pcf):	62.43		

SAMPLE AND SOIL TYPE

Boring No.:	EB-2	EB-2	EB-2	EB-3	EB-3			
Sample No.:	A	A	B	B	B			
Sample Depth (feet):	21.00	26.00	35.50	21.00	26.00			
USCS Soil Type:								
Specific Gravity:	2.70	2.70	2.70	2.70	2.70	2.70	2.70	2.70
Soil Description:	OLIVE GRAY LEAN CLAY	OLIVE GRAY LEAN CLAY W/ORGANICS	OLIVE GRAY FINE SILTY SAND	OLIVE GRAY LEAN CLAY	OLIVE GRAY LEAN CLAY			

DENSITY

Number of Rings:	6	6	3	6	6			
Wet Weight of Sample and Rings (g):	1103.3	1096.4	530.2	1116.2	1094.4			
Sample Diameter (in):	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4
Sample Height (in):	6.0	6.0	3.0	6.0	6.0			
Total Ring Weight (Tare) (g):	267.0	267.0	133.5	267.0	267.0	0.0	0.0	0.0
Dry Unit Weight (lbs/cu.ft):	89.71	86.19	90.42	92.94	86.76	#DIV/0!	#DIV/0!	#DIV/0!

MOISTURE CONTENT

Dish (Tare) No.:	26	210	233	236	215			
Weight of Wet Soil and Dish (g):	332.1	322.1	272.8	320.4	301.9			
Weight of Dry Soil and Dish (g):	266.7	252.6	231.3	261.3	235.8			
Weight of Dish (Tare) (g):	54.6	54.4	52.0	52.0	40.5			
Moisture Content (% of Dry Weight):	30.83	35.07	23.15	28.24	33.85	#DIV/0!	#DIV/0!	#DIV/0!

OTHER PROPERTIES

Moist Unit Weight (pcf):	117.38	116.41	111.35	119.19	116.13	#DIV/0!	#DIV/0!	#DIV/0!
Saturation (%):	94.73	99.06	72.33	93.71	96.93	#DIV/0!	#DIV/0!	#DIV/0!
Porosity (%):	46.78	48.87	46.35	44.86	48.53	#DIV/0!	#DIV/0!	#DIV/0!
Volumetric Water Content:	0.4431	0.4841	0.3353	0.4204	0.4704	#DIV/0!	#DIV/0!	#DIV/0!
Void Ratio:	0.8788	0.9557	0.8640	0.8136	0.9427	#DIV/0!	#DIV/0!	#DIV/0!

Tested by:	TG	Date:	Comp by:	TG	Date:

APPENDIX B

SESOIL MODELING INPUT AND OUTPUT